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Äspö Hard Rock Laboratory

Groundwater flow and solute transport modelling with support of chemistry data

Task 5

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Commissariat á l'Energie Atomique, France

September 2000

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Abstract

This report is part of the work performed for ANDRA concerning flow and transport mechanisms in natural fractured media.

We present here the contribution of CEA/DMT to Task 5 of the TASK FORCE SKB. This task aimed at integrating groundwater flow models as well as hydrochemical mixing models for the situation at the Äspö site during the excavation of the tunnel and shafts.

The work performed includes modeling the hydraulic problem as well as the transport and mixing of different types of water within the conducting features at the site. The calibration approach followed corresponds to looking for a best solution to the problem and include sensitivity analysis to appreciate the uncertainties in the calibration procedure.

However, since CEA/DMT only joined the Task 5 in April 1999, the work performed could only include partial calibration and sensitivity analysis for the different parameters of the system. Further work is required mainly for the transport part of the model.

Results for the hydraulic problem show that hydraulic data provided (conductor domain geometry, transmissivities, boundary conditions) are fairly consistent. Density effects connected with salinity proved important for deeper parts of the model and should be modeled.

Incorporation of transport data allows for further refinements of the model although transport parameters as well as mixing proportions data involve large potential uncertainties. Preliminary results show that the system is sensitive to parameters like initial and boundary conditions as well as transport parameters (particularly dispersion coefficients). This should be taken into account in the calibration strategy as well as in the discussion about the global consistency evaluation of the modeling.

Sammanfattning

Denna rapport utgör en del av det arbete som utförts på uppdrag av ANDRA rörande flöde och transportmekanismer i naturliga, sprickiga medier.

Vi presenterar här CEA/DMTs bidrag till Task 5 i SKBs Task Force. Denna uppgift syftade till att integrera modeller för grundvattenflöde och modeller för hydrokemisk mixning under de förhållanden som rådde i Äspölaboratoriet under tillredning av ramp och schakt.

Arbetet som gjorts inkluderar modellering av de hydrauliska problemen och transport och blandning av olika vattentyper i de vattenledande strukturerna på platsen. Kalibreringen följde principen att nå bästa lösning på problemet, och inkluderade känslighetsanalys för att utvärdera osäkerheten hos kalibreringsprocessen.

Men, eftersom CEA/DMT kom med i Task 5 så sent som i april 1999, kunde arbetet endast inkludera delar av hela kalibreringsarbetet och endast känslighetsanalys av vissa parametrar i systemet. Ytterligare arbete behövs beträffande transportdelarna i modellen.

Resultat från studien av det hydrauliska problemet visar att de hydrauliska data som presenterats (vattenledande strukturens geometri, transmissivitet, randvillkor) är tämligen stabila. Densitetseffekter, som är beroende av salthalten, visade sig vara betydelsefulla för djupare delar av modellen, och bör modelleras.

Användning av transportdata leder till ytterligare förfining av modellen, även om transportparametrar och data om blandningsproportioner medför stora, potentiella osäkerheter. Preliminära resultat visar att systemet är känsligt för sådana parametrar som start- och randvillkor samt transportparametrar (speciellt dispersionskoefficienter). Detta ska beaktas i kalibreringsstrategin liksom i diskussionen av den globala utvärderingen av modellens konsistens.

Contents

Chapter 1

Introduction

The TASK5 is part of SKB Task Force work performed at the Äspö site in Sweden. The Äspö site has been studied for several decades and is now one of the most precisely characterized site.

The specific objectives of this task are according to [*Wikberg 98*] :

- Assess the consistency of groundwater flow models and hydrochemical mixing reaction models through integration and comparison of hydraulic and chemical data obtained before and during tunnel construction.
- Develop a procedure for integration of hydrological and hydrochemical information which could be used for disposal site assessment.

The interests of CEA/DMT for this Task are mainly the following : Working at Äspö is a unique opportunity to test models against reality. Indeed, the quality as well as the volume of the data set is such that a rather precise and realistic modeling can be undertaken: several water conducting features are described, whereas hydrological, transport and geochemistry tests have been performed. The actual status requires modeling of flow and transport processes as well as a calibration procedure and evaluation of the importance of the different types of data as well as global consistency check of the modeled system.

Nevertheless, since CEA/DMT joined the task in the middle of 1999, lacking any kind of background of Äspö at the site scale, the work performed could not reach the above mentioned level. Indeed, the results are preliminary in the sense that the calibration procedure including a sound sensitivity analysis for the different parameters could not be brought into the transport model.

Chapter 2

Modeling work performed

The work follows the requirements as well as the data provided within the Task Force and the deliveries [*Äspö Task Force*]. The modeling tool is CASTEM2000 developed at the CEA/DMT [2].

CASTEM2000 is a general multi-purpose finite element code devoted to studies in structural mechanics, fluid mechanics and thermics (see reference CASTEM2000 [2]). Concerning the applications for the Waste Repositories, the code covers the following scientific fields : Hydrogeology, Thermics, Rock and Soil Mechanics, Geochemistry, and the following couplings : Transport-Geochemistry, Thermo-Hydraulics, Hydro-Mechanics, Thermo-Hydro-Mechanics.

CASTEM2000 belongs to the class of "object oriented" codes. It is structured as a "library" of operators acting on objects. These operators may be: i) differential, such as a gradient, a laplacian, a time derivative, ..., for the solution of a transport equation for instance; ii) geometrical, such as segmentation of a line in a number of equal segments, for the meshing operations; iii) logical, etc. The objects may be scalar, vector, tensorial fields, or parts of a meshing, or more simply files. More generally they are appropriate to the concepts manipulated by engineers. A macro-language allows the common user to manipulate the operators and objects. One of the principal advantages of this structure is that the operators are independent basic bricks and not dedicated to a particular application. It is the common user which assembles the operators in order to solve his particular problem. If the operator does not exist it may be developed by the user.

The available spatial discretization formulations are standard Galerkin finite element and mixed hybrid finite element. The geometry may be 1D, 2D, 3D and axisymetric. The time discretizations schemes are the standard ones (explicit, implicit, ...). Pre-processors (meshing for example) and post-processors (graphics, ...) are parts of the code. Couplings with other codes are possible.

2.1 Geometrical features

The conductor domains alone are here taken into account. The matrix blocks could be integrated in further modeling steps, their importance for transport problems being potentially important.

The geometry of the fractures is taken explicitly into account in the meshing. From the initial 21 fractures provided in the deliveries, 16 remain in the model : EW1S, EW3, EW7, NE1, NE2, NE3, NE4N, NE4S, NNW1, NNW2, NNW3, NNW4, NNW5, NNW6, NNW7, SFZ11. The other ones were eliminated as they don't take part in the flow when matrix blocks are not modeled (not intersected by tunnel and shaft or connected to an intersected fracture).

The domain size is 2km x 2km x 1km as provided in the deliveries.

Practically speaking, the geometrical features are treated as 3D objects as required by the present version of CASTEM2000. We proceed as follows.

1. Hydraulic conductors domains are first obtained as 2D objects from an automatic mesh generator : IDEAS. Locations corresponding to intersections are identified.
2. 3D features are generated from these plans by translation : a depth is affected. In this operation, nodes located at the extremities of these units, corresponding to an intersection with another conducting feature are identified. The elements generated are prismatic. The geometry for the tunnel and shafts was obtained by 'digging' 3D features into the hydraulic conductor 3D domains generated.
3. The intersections are not discretized. The final geometrical model consists of 16 3D units corresponding to the conducting features retained here, as well as a system of relations providing the connectivities at the extremities of these 16 units. These are necessary for the modeling of flow and eulerian transport since continuity relations are imposed based on them.

The following comments are necessary to understand this geometrical model and how it can be operational. A classical option would be to model the conducting features as 2D units. This would be of no use here since the version of the code we worked on did not allow 2D modeling within 3D problems. The next idea consists of a fully 3D model. The meshing of some fracture intersections proved cumbersome due to the relative extensions of the meshes. So, intersections were not meshed geometrically but continuity of flow and transport variables was imposed at fracture intersection within the simulation procedure. This continuity is achieved by a classical Lagrangian multipliers method. A drawback of this strategy is nevertheless that particle tracking procedure provided in the code could not be used since no geometrical continuity exist between the fractures.

The tunnel is represented by a prismatic element (diameter around 80m) where boundary conditions are imposed. A skin effect is introduced in the first mesh on the tunnel side. This effect represents two phenomena : first, grouting which was employed during the excavation to limit the inflow of water into the tunnel, second, the accurate diameter of the tunnel is not directly modeled here but by means of introducing a resistance accounting for the drawdown over this distance.

6514 meshes are required to represent this system including tunnel and shafts.

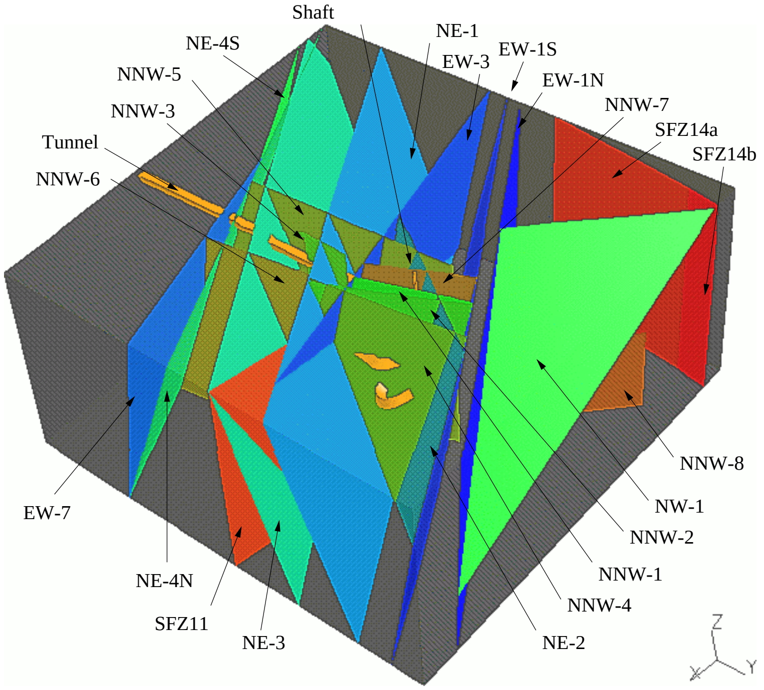


Figure 2.1: Hydraulic conductors, shaft and tunnel. Domain size 2km x 2km x 1km

At the present state, only the fracture network is considered. Further plans could include modeling of the matrix blocs by means of a domain coupling procedure. This procedure (domain decomposition) should prove interesting for two reasons at least :

- Kinetics for flow and transport in the considered domains (fracture network and matrix blocks) are very different. As such, very different time and space discretisation strategies are required. In particular, modeling the whole system as a single domain (so with a common time step) would require very fine discretisation (at least in the blocks towards the fracture interface) to guaranty a good dynamic estimation of the transport mass exchanges between both domains. Such a requisite imposes a special procedure (potentially difficult) for the discretisation of the system and can lead to a large number of meshes. Former studies proved that coarse meshing across the interfaces lead to over estimation of matrix diffusion processes (several tenth of percents) as well as a false dynamic (temporal) response of the blocks.

- Domain decomposition potentially leads to saving computer time since resolution on smaller sub domains are chained and several time steps can be done for one subsystem for only one for the other.

Nevertheless convergence has to be obtained for the problem treated.

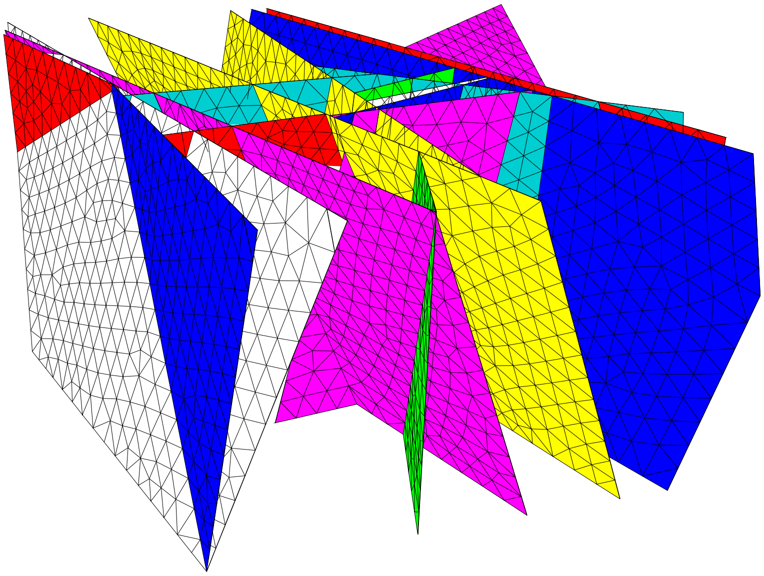


Figure 2.2: Hydraulic conductors

2.2 Models and numerical aspects for flow and transport

The work is performed within the CASTEM2000 code [2]. In relation with the present task, CASTEM2000 allows for the following modeling. One may refer to [*Dabbene 98*], [*Dabbene 94b*] and [*Dabbene 95*].

- Stationary and transient flow.
- Transport of concentration fields by advection and dispersion, diffusion.
- Coupling between flow and concentration transport to account for density effects.
- Particle tracking procedure.
- Geochemistry including coupling with transport.

From these, only the 3 functionalities were employed in the present study. Particle tracking was not used because the geometry generated could not fit the requirements for particle tracking : as mentioned before, the geometry of the intersection is not explicitly taken into account. The continuity of the different fields is guaranteed for the intersections by imposing relations within the code by Lagrangian multipliers. As such, the requirement of producing advective travel times and travel paths to the control points would require another method. This difficulty was circumvented by back transporting pulses of concentration from the control points and follow the maximum of the plume. This method produced somewhat inaccurate results for reasons stated below. No geochemistry is modeled here.

The equations solved for the flow and transport problem are the following (one may report to [*Rhen et al. 97*] or classically to [*de Marsily 86*]) :

For the Darcy velocity :

$$\rho\vec{U} \; + \; \frac{K}{g}\left[\vec{\nabla}P + \rho g\vec{\nabla}z\right] \; = \; 0 \tag{2.1}$$

- K hydraulic conductivity (m/s) ;
- g gravity coefficient (m/s^2) ;
- z altitude (m) ;
- ρ (kg/m^3) ;
- $\vec{U}$ Darcy velocity(m/s) ;
- P total pressure (Pa).

Mass conservation is expressed as :

$$C_H.\frac{\partial p}{\partial t} \; + \; \vec{\nabla}.\rho\vec{U} \; = \; 0 \tag{2.2}$$

With $C_H = S/gb$, S for storativity (-) and b for fracture opening (m).

Transport equation for the concentration fraction χ is given by :

$$\frac{\partial\omega\chi}{\partial t} \; + \; \vec{\nabla}.\chi\vec{U} \; = \; \vec{\nabla}.\left[(D^* + \bar{D})\vec{\nabla}\chi\right] \tag{2.3}$$

- ω porosity (-) ;
- D^* diffusion coefficient (m^2/s) ;
- $\bar{D}$ dispersivity tensor (m^2/s) is here diagonal in the local velocity base ; ($D_l = \alpha_l|U|$ for the longitudinal dispersivity (m^2/s) and $D_t = \alpha_t|U|$ for transversal dispersivity (m^2/s)). α_l et α_t coefficients (m).

The resolution is performed by Mixed and Hybrid Finite Element method. This method, which respects mass conservation, provides good quality flow and concentration fields (continuity and conservation of the mass) for heterogeneous situation commonly encountered in natural formations [*Chavent and Jaffré 86*]. Let us remind that this formulation solves simultaneously the flux equations (Darcy flow and mass flux) and the mass balance equation (head and concentration).

Full implicit schemes are used for flow and transport problem.

For the simulation provided, around 7000 meshes were required, 200 time steps were used for the flow problem (basic time interval is around 20 days) and was refined for the transport problem. The flow problem includes transient boundary conditions and requires around 1 CPU hour.

The type of modeling considered for the intersection (not meshed but continuity of the solution imposed by means of Lagrangian multiplyers) requires two comments :

- This leads to neglecting the size of the intersection volume. This is nevertheless considered to be not important here compared to the uncertainties in the position of the conductor domains.
- For the eolian transport modeling, continuity of concentration at the intersection means complete mixing, classical assumption which is made throughout the study.

In order to take fully coupled salinity density effects into account, transport calculation is required and coupling is done by an iterative method between both equations. In this case, simulation of coupled flow requires more than ten hours of CPU for good convergence. This is why a limited number of coupled simulations were performed, the calibration procedure being fulfilled taking only permanent density effects into account. Fully coupled density effects were then later added to the selected optimal calibrated model to study their influence. Transport calculations require around 4 hours.

The boundary conditions for the flow problem are taken from the regional model by [*Svensson 97*] (*delivery 11*) including pressures as well as salinity fields. No flow is considered for the bottom limit of the model. Limited recharge is taken for the Äspö geometry (from 5 mm/year to 0) and imposed pressures are considered for the Baltic sea. Atmospheric pressure is imposed in the tunnel and shafts as the excavation proceeds. Inflows into the tunnel are simulated and compared to the measured ones towards calibration. Drawdowns measured in different boreholes are incorporated into the calibration procedure as well.

For the transport of 4 types of waters, the initial and boundary conditions are taken from the interpolation results by M3 provided in data *delivery 7*. Two types of boundary conditions were considered, the one corresponding to the situation before and after tunnel construction.

2.3 Calibration phase

Due to our late arrival in the Task5 of the Task Force, only a limited amount of data has been taken into account. These involve :

- Natural flow at the site before excavation with comparison with the results by [*Svensson 97*].
- Inflow in the tunnel during the excavation as well as drawdown in the different boreholes intersecting the fracture network : KAS02, KAS04 to KAS09 and KAS13 and KAS14. The hydraulic calibration encloses hydraulic characteristics of the fractures: mainly fracture transmissivity and grouting. Storativity could not be calibrated due to the shape of the measured signals.
- No proper calibration of the transport characteristics was done due to a lack of time. The data taken into account are mixing proportions of the waters at the control points by M3 modeling (cf. *delivery 15*). Elements of a sensitivity analysis are provided below.

The rationale behind this calibration phase is looking for a single *best solution* taking the data provided into account and then conduct sensitivity analysis to evaluate the importance of each parameter as well as the uncertainty associated.

The figures corresponding to the results are provided in section 3.

2.3.1 Flow problem

Only data from natural flow conditions as well as tunnel construction have been taken into account. The tests related to LPT2 have not been used.

We used the geometry of the hydraulic conductors provided in the data deliveries (see section 2.1). So calibration corresponds to choosing transmissivity as well as storativity values to be associated to the hydraulic conductors as well as values for grouting associated with each hydraulic conductor domain ([*Rhen et al. 97*], page 159). A constant transmissivity as well as quantity of grouting is considered per conductor domain. The calibration was made by trying to come to fitting the tunnel inflow data as well as the pressure measurements within the boreholes KAS02, KAS04 to KAS09 and KAS13 and KAS14. The inflow into the tunnel proved to be the most sensitive to the transmissivity, the pressures along the boreholes less sensitive. From a practical point of view, for each tunnel section, contributions corresponding to the different conductor domains involved were drawn (see section 3) and transmissivities adjusted for the conductor domains playing a dominant role. The drawdown measured at the boreholes locations proved in agreement. This leads us to the conclusion that the system is globally consistent.

In a first row of simulations we made an attempt to achieve a calibration without considering grouting. We could thus reach a rather consistent solution (compared with the data provided) by reducing the transmissivity values associated with major conducting features like NE1 and NE3. Nevertheless, grouting was introduced during the progress of the excavation to limit the inflows into the tunnel. It is as such necessary to take this effect into account. Since only grouting volumes are provided and not permeabilities for instance, this quantity is determined within the calibration procedure. The respective importance of grouting for each location is taken into account. Grouting is considered for the conductor domains NE1 and NE3 (compare with the data from [*Rhen et al. 97*], page 159), no grouting being introduced for the other conductors domains in the model. These locations indeed correspond to the major inflow rates in the modeled system. From the point of view of the calibration procedure, the sensitivity to the transmissivities in these conductor domains was reduced.

This calibration procedure aims here at a single *best solution*. Nevertheless, there is not unicity of this solution. We proceeded based on the contribution of each conductor domain to the total inflow. The transmissivities corresponding to the conductor domain playing a major role in the total inflow were changed whereas the others were kept at the same value. This procedure provides direct insight into the sensitivity of the system to transmissivities associated with each conductor domain. For instance, results are very sensitive to the transmissivity values associated to the main conductors, whereas transmissivities associated to minor ones can't be determined within an order of magnitude based on the flow problem calibration.

The transmissivity values affected to the conductor domains are provided below (Tab. 2.1 and Fig. 2.3), grouting was chosen on the basis of the data available ([*Rhen et al. 97*], page 159) and associated to NE1 and NE3.

Conductor domain	Transmissivities proposed $(*10^{-6}m^2/s)$	Transmissivities calibrated $(*10^{-6}m^2/s)$
EW1S	12.	12.
EW3	17.	13.6
EW7	15.	12.
NE1	220.	220.
NE2	.12	.80
NE3	320.	300.
NE4N	31.	25.
NE4S	31.	31.
NNW1	8.6	1.1
NNW2	24.	3.
NNW3	20.	20.
NNW4	65.0	11.5
NNW5	4.	4.
NNW6	14.	14.
NNW7	7.5	5.
SFZ11	3.6	3.6

Table 2.1: Transmissivity values associated to the conductor domains, before and after fit

As mentioned, the consistency of the calibration with the above mentioned data is fairly good. Only minor changes within the transmissivity values were required in order to achieve good fits. An exception of limited importance should nevertheless be mentioned: satisfactory calibration for conductor domain NNW4 would have required stronger contrasts in the levels of grouting associated to the different portions where the tunnel meets this conductor domain. It would have been necessary to introduce a variable transmissivity field within the conductor domain or alternatively modify the geometry of the conductor domain. This has not been done here and might have consequences for the quality of the predictions provided in the following.

Boundary conditions were kept constant here according to the regional model by [*Svensson 97*]. No sensitivity analysis to boundary conditions was conducted. Nevertheless an effect introduced by imposing boundary conditions at a finite distance was observed when considering the inflows into the main East West conducting features : these units receive more inflow from the sides of the calculation domain closest to the tunnel, and less from other directions. This introduces a bias which was not further studied.

Storage coefficients were kept according to the values provided by [*Rhen et al. 97*] in the formula relating transmissivity and storage coefficient (page 214). The data show a very quick response in terms of inflow when crossing a conducting domain. Furthermore,

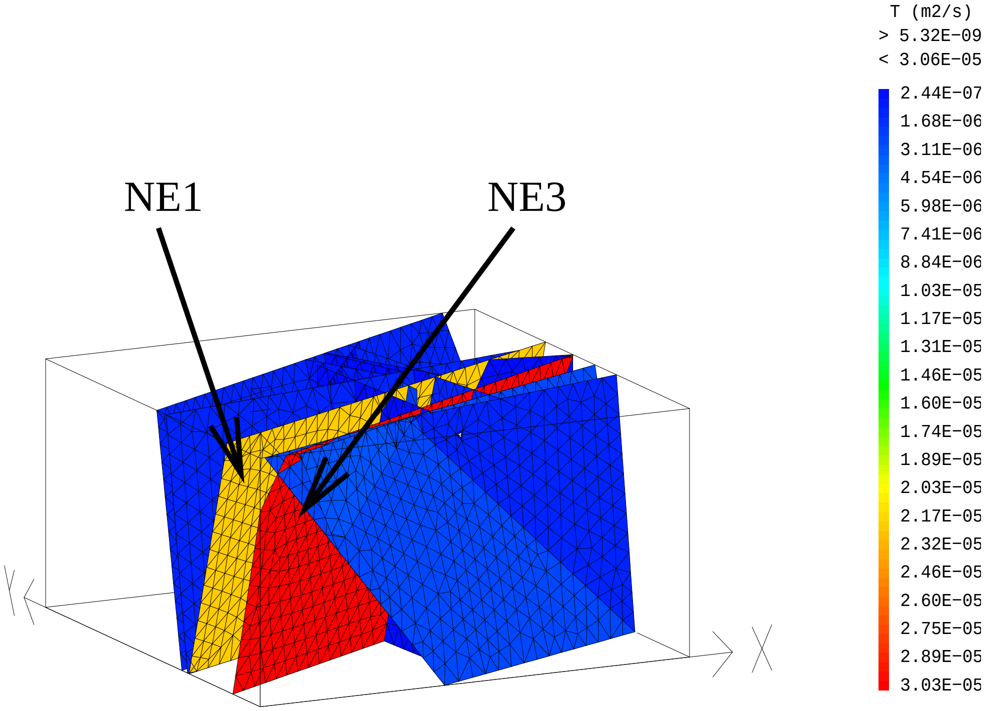


Figure 2.3: Transmissivities calibrated for the conductor domains

some of the curves show that the conductor domain apparently consists of different fractures spreading larger than the actual fracture size modeled. Indeed, the real fracture reacts quicker and some time after the modeled fracture in a way that can't be accounted for by a storativity effect. As a consequence, the simulations done used a time step around 20 days leading to series of quasi permanent calculations.

Further calibration steps would anyway be necessary. Figure 3.11 shows increasing drawdown differences for large times. This increase probably has two main reasons. First, total inflow in the system decreases as the tunnel excavation has already reached its end. This is probably due to additional grouting in the tunnel and shafts which is not considered in our model. Second, calibration should be improved, especially for deeper control points reached at later times of the excavation.

2.3.2 Transport problem

Transport of salinity and importance of density effects

We firstly made simulations limited to transport of salinity before we moved on to transport of four types of water for simulations for mixing proportions. These simulations are based on the data taken from regional model by [*Svensson 97*] providing initial conditions as well as boundary conditions. They provide the basis for coupled modeling of density effects. No calibration was attempted for the salinity.

A comparison was conducted for the parameter set corresponding to the *best solution* obtained from the hydraulic calibration phase. Three types of simulations were made to address the issue of density effects :

- Simulation including full coupling between flow and transport of salinity field.
- Simulation without coupling : the initial salinity field is not transported so that permanent density effects are treated for the flow problem.
- Simulation without any density effect (freshwater is considered).

Globally, the excavation creates a depression collecting water from all around. This leads to transport of the different types of waters towards the tunnels and shafts. This includes freshwater from to below Äspö, low salinity water from the Baltic Sea at the top of the modeled domain, higher density saline Glacial water from the sides of the model and brine water from the deeper parts of the domain.

The calibration phase has been conducted based on simulations including permanent density effects (i.e. without coupling) in order to reduce the computer time. As mentioned before, the study of the importance for density effects has been conducted for this calibrated transmissivity parameter set.

Results show that density effects are of weak importance for the flow problem (in terms of inflow into the tunnel as well as pressures in the boreholes). The excavation of the tunnel causes the major perturbation and density effects are side effects.
This is not true for the transport of waters. Mixing proportions obtained for a full coupling simulation and for a freshwater calculation show, as a global rule, weak differences for control points close to the surface (typically CP2, CP3, CP4, CP6) whereas larger differences in water proportions (roughly at the order of 10%) can be found for deeper control point locations (CP8, CP9, CP11). More detailed interpretations for these results are not straightforward and would require further analysis. However, only slight differences in the mixing proportions could be found between full coupled calculations and simulations taking permanent density effects into account.

So, for the range of parameters considered for this *best solution*, and for the initial and boundary conditions of salinity extracted from [*Svensson 97*], it appears that density effects should preferably be taken into account in the simulations and that permanent density effects are sufficient.

A further comment on this result is that discrepancies in mixing proportions are comparable here (between simulation with and without density effects) to what could be found in the preliminary sensitivity analysis reported below concerning the influence of boundary conditions. This means among others that a sound calibration procedure for the whole system should should rely upon a good match of salinity data.

Mixing of waters

We provide in the following simulations for transport problem taking four waters into account. These were taken in agreement with the reference waters from [*Rhen et al. 97*] and the data deliveries : Meteoric, Baltic, Glacial and Brine. The initial condition as well as the boundary conditions are taken from the interpolations with M3 to be found in data *delivery 7*. The data to be matched are taken from the same *delivery 7* and involve the control points provided in data *delivery 15*. Among those points the ones corresponding to the conductor domains were retained. The list is provided in table 2.2. Boreholes locations in a close vicinity are not distinguished.

Control point number	Borehole
CP 2	SA0813B - SA0850B
CP 3	SA1327B - SA1229A - KA1061A
CP 4	SA2074A
CP 5	SA2783A
CP 6	KA1755A
CP 8	KA3110A
CP 9	KA3385A
CP 10	KAS03
CP 11	KAS07

Table 2.2: Control points considered and corresponding borehole references

Due to a lack of time, no calibration has been fulfilled. The hydraulic parameters were obtained from the previous hydraulic calibration phase. The transport parameters including fracture apertures (or porosities) as well as dispersion coefficients are taken from [*Rhen et al. 97*], section 8. These quantities are as follows :

- *Fracture apertures* are introduced as porosities in the model. The aperture values are chosen according to the equation relating to the transmissivity : $e = 1.428T^{0.523}$ in [*Rhen et al. 97*].
- Rules for the *dispersivity values* are provided by [*Rhen et al. 97*], page 404. We took here dispersivity values comparable to the size of the elements of the mesh, which is roughly 50 m for the longitudinal component and 10 m for the transverse component. No sensitivity analysis to this parameter was conducted although it plays a potentially large role as stated below.

The results provided here date back to the prediction results delivered in December 1999. Due to a lack of time, further calibration steps were not fulfilled. These steps would nevertheless be necessary to refine the model. The strategy planned included calibration considering M3 mixing proportion results as reference 'measurements'.

Preliminary results show that transport results seem to help refining the model. This is based on the single fact that the best fit in terms of inflow in the tunnel and drawdowns in the boreholes provided better fit for the mixing proportions as was obtained in a former simulation based on the transmissivity values initially provided (prior to hydraulic calibration). This very preliminary observation goes in the direction of consistency of the model towards data used for hydraulic and transport calibration.

We provide in the following more precisions about the way such a calibration procedure could be fulfilled based on preliminary sensitivity analysis made.

A general trend in the results obtained against M3 mixing proportions is the following: Meteoric water proportion is too important for shallow control points whereas Glacial fraction should be increased for deeper control points.

A first step calibration strategy could there involve several categories of parameters :

- Hydraulic parameters : transmissivities and grouting quantities associated to the conductor domains. Preliminary results showed nevertheless that sensitivity is rather weak for the transmissivity sets considered which were calibrated on the flow problem.
- Transport parameters : transport apertures, dispersivity (uncertain data).
- Transport boundary and initial conditions (obtained with uncertainties associated by M3 modeling on a rather rough grid).

The influence of these parameters is potentially important. Among them, boundary conditions are potentially important since advective travel times are rather quick for control points in the vicinity of the surface as shown below from back tracking analysis. To our opinion the dispersivity values considered might prove important as well. This is based on the fact that we firstly conducted a simulation considering isotropic dispersivity which lead to slightly different results in terms of mixing proportions from the base case reported here (lateral dispersivity being one fifth of the longitudinal).

Another direction of research for calibration could include refinement of the model, especially :

- Achieve a better description of flow in the vicinity of the surface : in particular, include a non saturated zone below Äspö limiting the Meteoric water inflows.
- Provide larger proportions of Glacial water by working on the initial and boundary conditions or on the geometry of the conductor domains (in oder to introduce new connections to the Glacial water reservoirs).

Uncertainties regarding the global system provide numerous acceptable ways of calibrating the system. The rationale of the calibration procedure which was not undertaken due to a lack of time, would be to obtain a best solution and provide ranges of accuracy by sensitivity analysis.

Back tracking for control points

We developed a procedure to simulate the travel times from the limits of the domain to the control points during the transient flow generated by the tunnel excavation. This procedure is not a typical back tracking procedure based on particle tracking. This could not be achieved here since conductor domains are not geometrically connected in our model but flow and transport is simulated imposing continuity of the fields at the interfaces.

So we developed a back tracking procedure based on concentration field back transport (eulerian approach) in the flow fields calculated previously. More precisely, travel times were obtained following the (back) motion of the maximum of a punctual initial concentration plume released at the control point. This procedure provided acceptable results though still unprecise. To our understanding, the roughness of the results is mostly due to boundary conditions effects : the number of meshes between the control points and the boundaries of the domain where a no diffusive flux condition is imposed is below 20. The procedure should prove more efficient for a refined meshing of the system (this was indeed planned but could not be achieved within the time frame provided).

The results obtained correspond to typical times for convective flow to reach the different control points. This value changes along the excavation procedure. The simulation correspond to back tracking from a time corresponding to the end of the excavation phase.

A general result is that travel times are rather quick for the control points close to the surface (weeks to months). The shallow control points connect with the ground level, whereas deeper control points connect with the sides of the modeled area (several months). This means that boundary conditions play an important role as reservoirs for the different water types quickly producing into the control points. As a consequence sensitivity to initial conditions as well as boundary conditions is required. These conditions are indeed taken from M3 calculations and include uncertainties.

Sensitivity to transport boundary conditions

Two boundary conditions in terms of mixing proportions extracted from M3 results were considered. Mixing proportions corresponding to conditions first before and then after tunnel excavation were considered. The results provided below, corresponding to the *best solution* involve the conditions before tunnel excavation.

Comparisons between both types of calculations show that the situations mostly differ for the compositions in upper types of waters, Baltic and Meteoric. This is not surprising since, as stated before, travel times to the tunnel in the upper part of the domain are rather quick. Anyway, the system is sensitive to the boundary conditions to a level of several percents mostly for these types of water (Baltic and Meteoric). Boundary conditions could as such be introduced into the calibration procedure. An other consequence is that interpolated boundary conditions should be considered in further steps of the modeling work.

Sensitivity to initial conditions was not studied here. The dependence is nevertheless potentially important, at least accounting for mixing proportions in the deeper parts of the modeled domain as well as for short time mixing proportions for shallow control points.

Sensitivity to dispersivity values

Dispersivity values used in the simulations of the transport of different water types are large as mentioned before in order to assure a good stability of the results. Peclet values are indeed of the order of 1. Consequences are that water concentration fronts are smoothed and mixing proportions are somewhat averaged. Due to a lack of time, no sensitivity study to this parameter was fulfilled. One point is nevertheless worth mentioning. In former preparatory steps for the transport simulation, isotropic dispersion was used: transverse dispersion was affected the same large value as that of the longitudinal dispersion. Comparisons were conducted for the same *best solution* data set resulting from hydraulic calibration. Results show large differences in the mixing proportions obtained, in the transitory as well as final permanent phase of the signals. This is mainly true for deeper control points. Further analysis would be necessary to find the rationale behind these results.

Nevertheless a point worth mentioning is that the amplitude of variations for the results are here maximal compared to other sensitivity analysis performed previously (boundary conditions, density effects). As a consequence, dispersivity should be incorporated into the calibration procedure and sensitivity analysis.

Perspectives on the transport problem

These results provide the following view on the problem of integration of hydraulic and transport data.

At the present level, mixing proportions help discriminate among several solutions acceptable from a hydraulic point of view. As such, transport data help further calibrating the system. Since only preliminary results could be obtained for the transport problem, it is not possible to assess the consistency of the transport side of the model towards the hydraulic part. Nevertheless, preliminary sensitivity analysis show that the system is quite sensitive to transport parameters which are uncertain (among others dispersivity values). This will limit the ability to conclude definitively for consistency of the different types of data.

Chapter 3

Results

We provide here with results from the best data set used, called previously the *best solution*. So, as stated before this data set corresponds to further steps in flow calibration but a primary step in transport calibration. In order to obtain a better solution model, further understanding of the transport mechanisms at the site is required (water travel time and origins, reliability of fracture transport apertures provided ...).

For all the figures provided, time origin corresponds to the start of the excavation of the tunnel : 1st october 1990.

All the results are provided on the geometry given in figure 3.1 where the tunnel, the island Äspö as well as the contours of the conductor domains are figured.

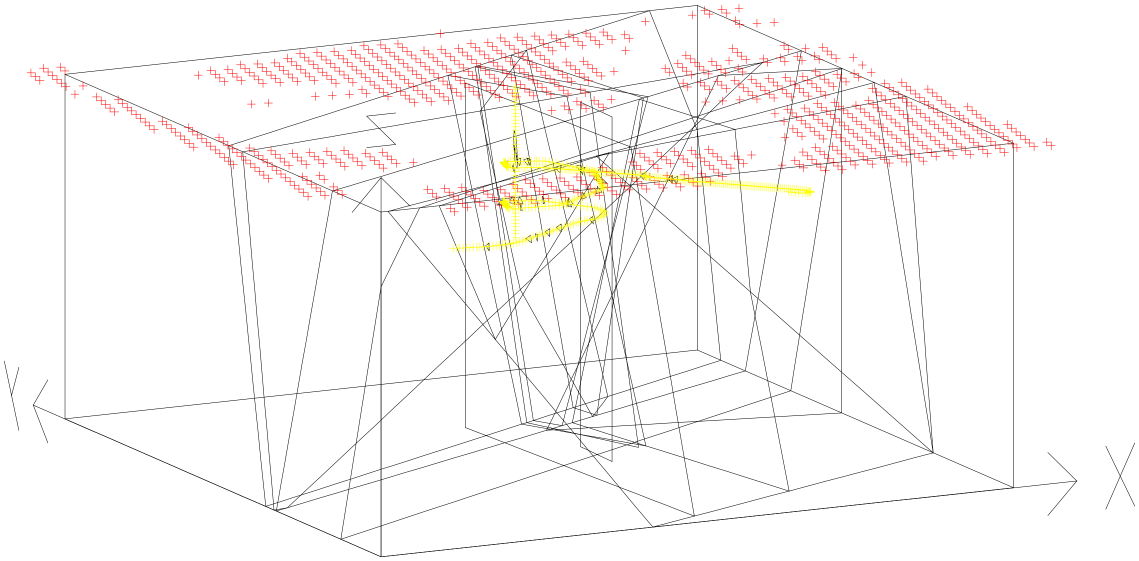
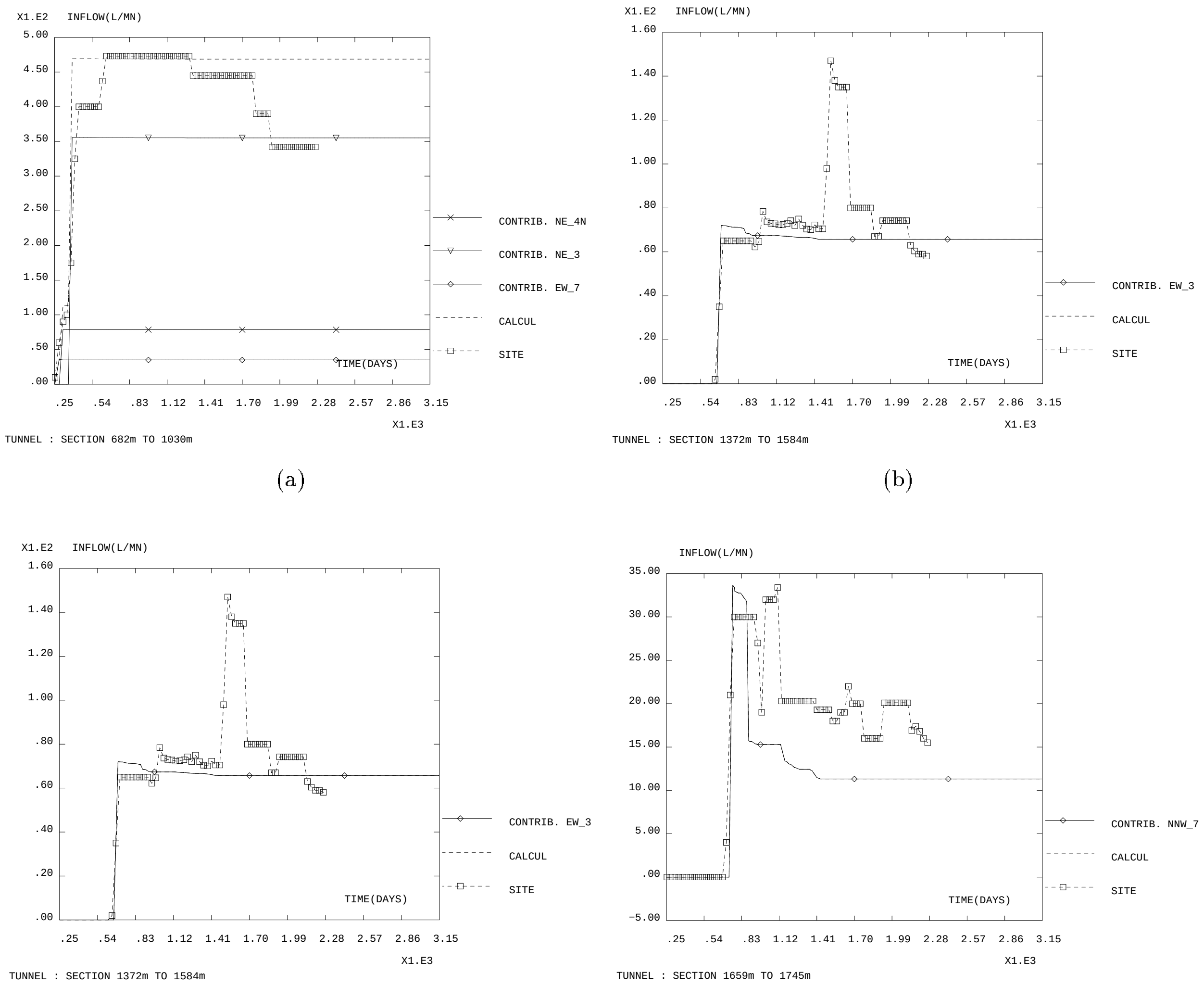


Figure 3.1: Geometrical features (Äspö, tunnel, conductor domains)

3.1 Water inflow into the tunnel

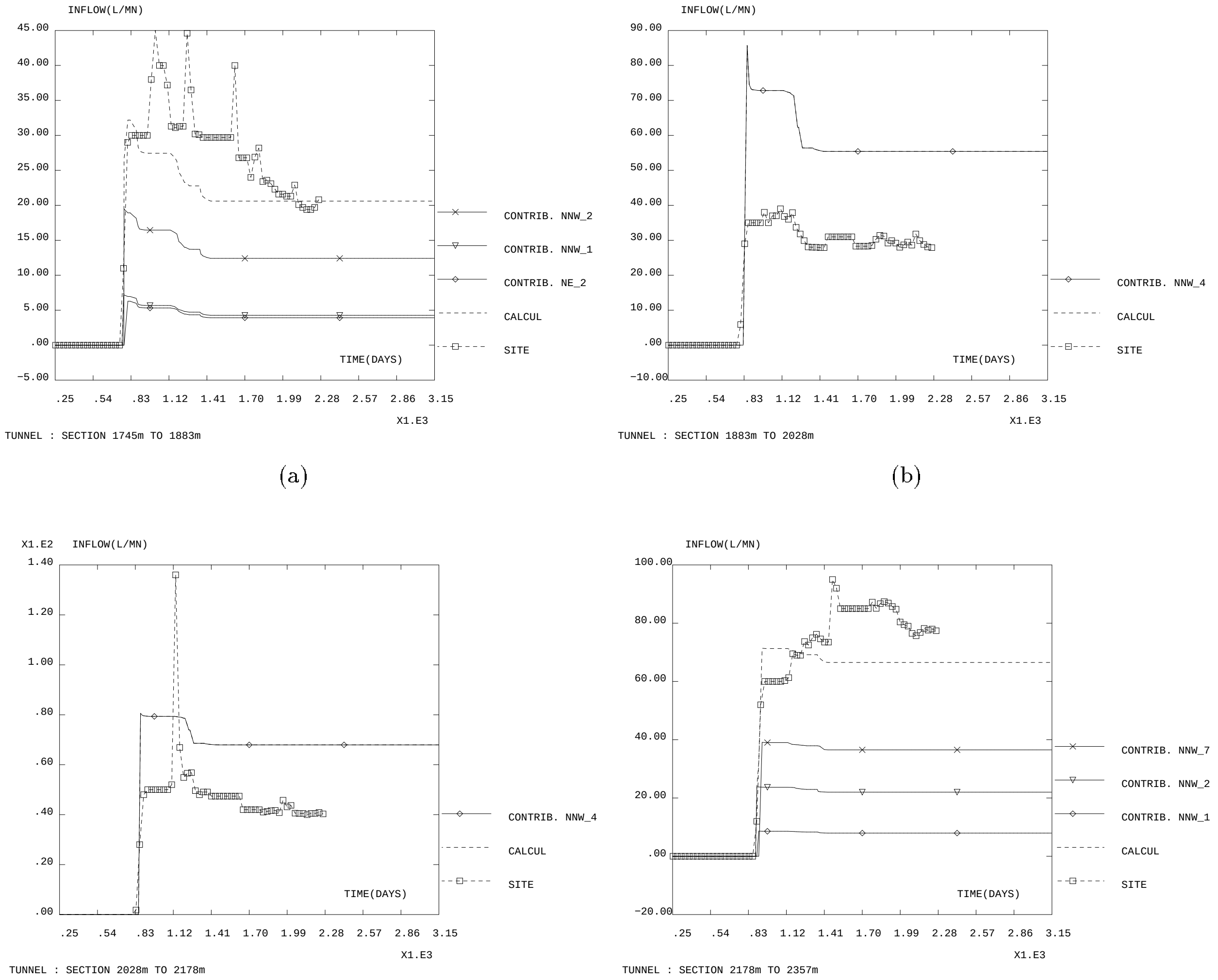
Water inflows in the tunnel proved very sensitive to the transmissivity and grouting and as such were more important that the pressures at the boreholes. As stated before, the calibration is consistent. The exception being for NNW4 for which different levels of grouting or a variable transmissivity would be required (cf. section 2.3).



(a) (b)

(c) (d)

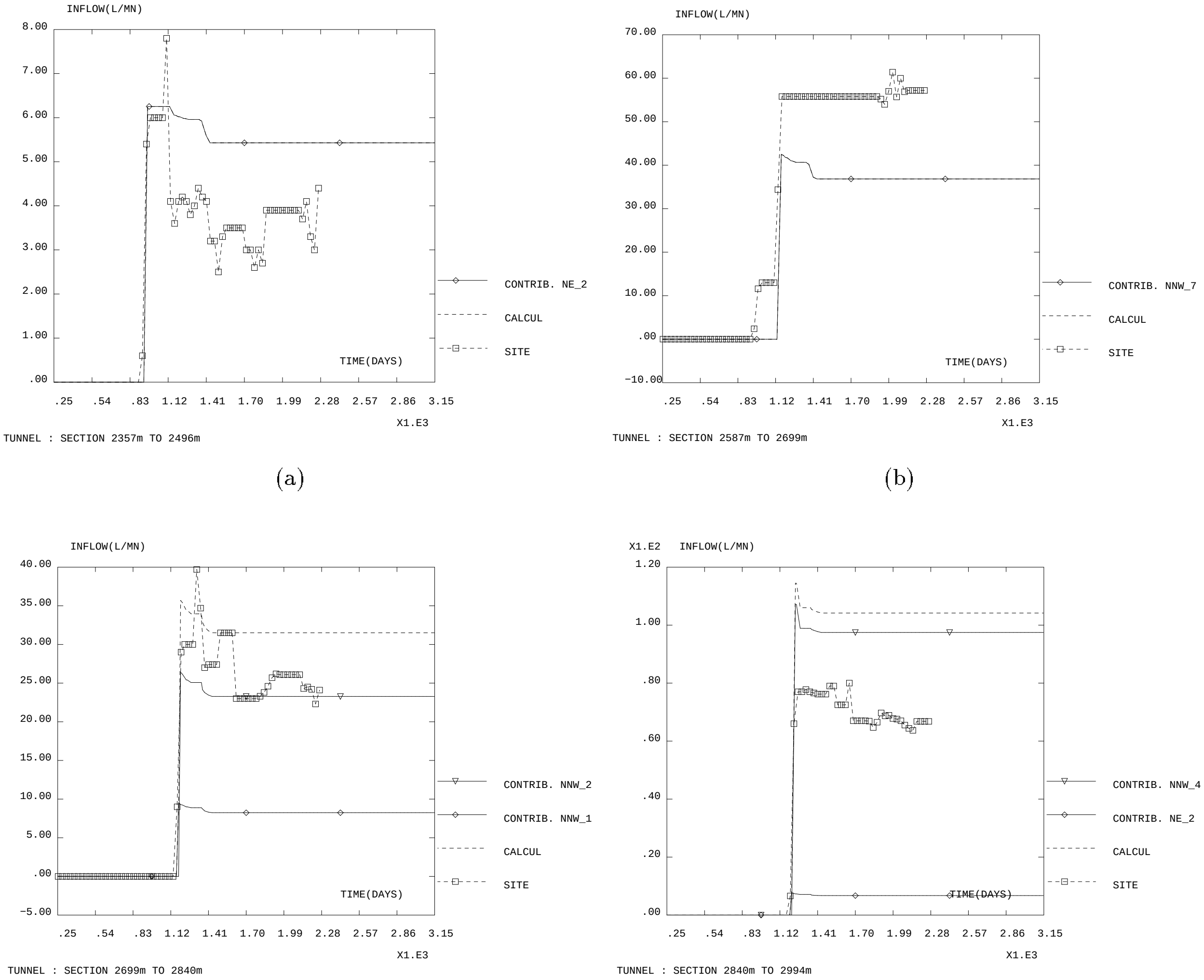
Figure 3.2: Inflows into the tunnel for different tunnel sections. Measured and simulated results as a function of time



(a) (b)

(c) (d)

Figure 3.3: Inflows into the tunnel for different tunnel sections. Measured and simulated results as a function of time



(a) (b)

(c) (d)

Figure 3.4: Inflows into the tunnel for different tunnel sections. Measured and simulated results as a function of time

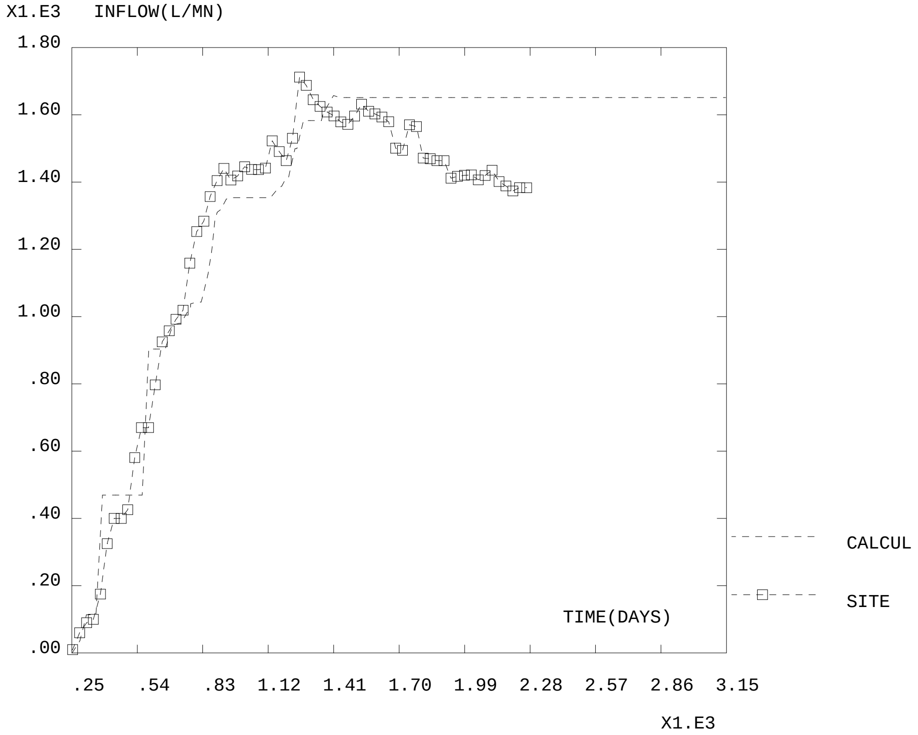


Figure 3.5: Total inflow into the tunnel and shafts as a function of time. Simulated and measured results

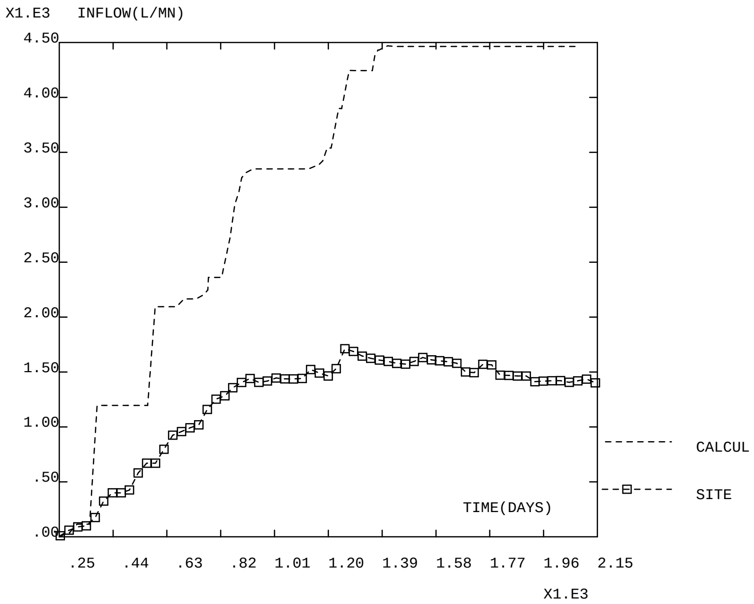


Figure 3.6: Total inflow into the tunnel and shafts before calibration. Simulated and measured results

3.2 Drawdown in the boreholes

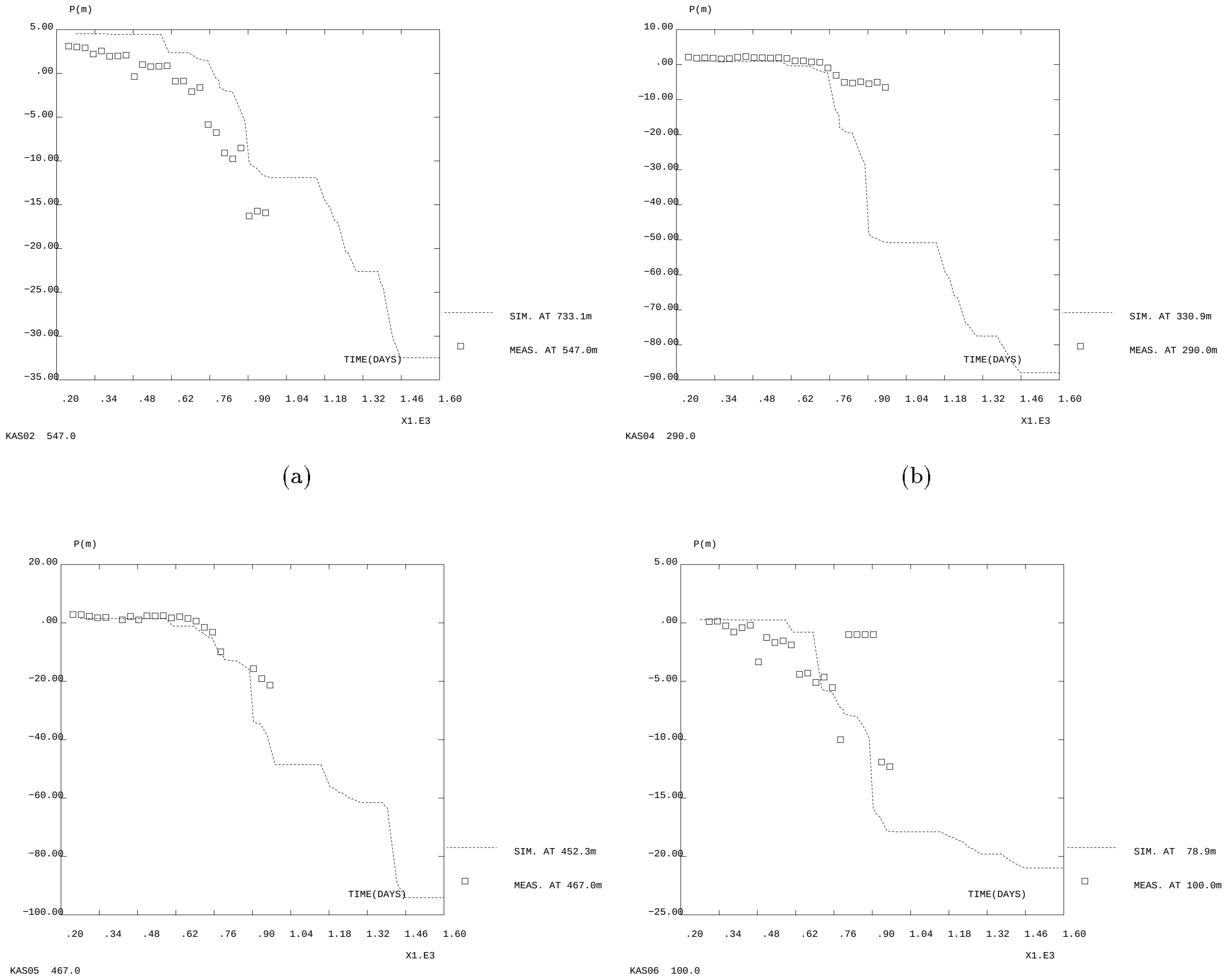
The expressions for the mean error (dh) and accuracy (Dh) provided on figure 3.11 are the following :

$$dh = \frac{\sum_{i=1}^{n}(h_i^m - h_i^c)}{n},$$

$$dh(abs) = \frac{\sum_{i=1}^{n}|h_i^m - h_i^c|}{n},$$

$$Dh = \sqrt{\frac{\sum_{i=1}^{n}(h_i^m - h_i^c - dh)^2}{n}},$$

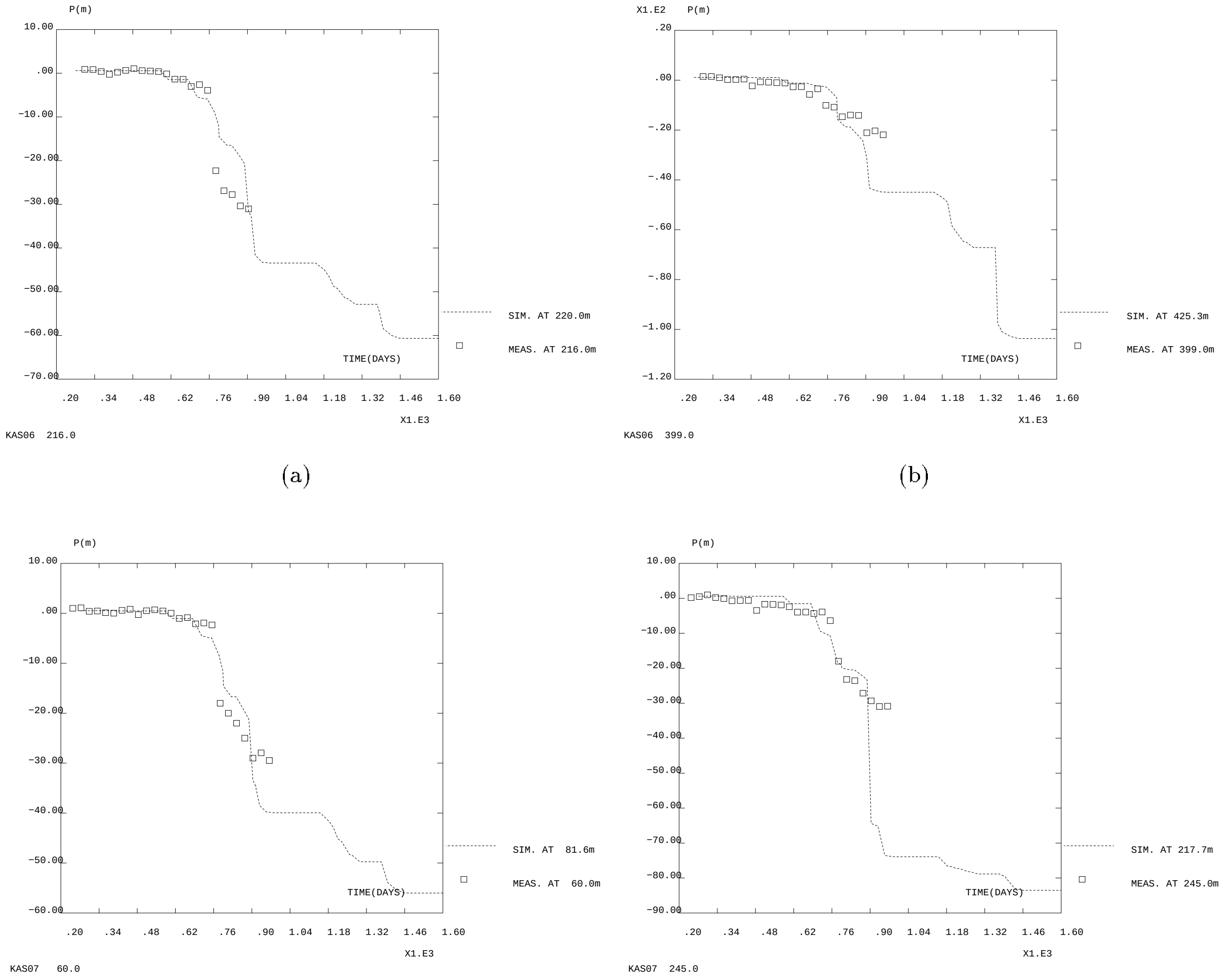
where n is the total number of measured values, h^c stands for calibrated head values, h^m for measured head values.



(a) (b)

(c) (d)

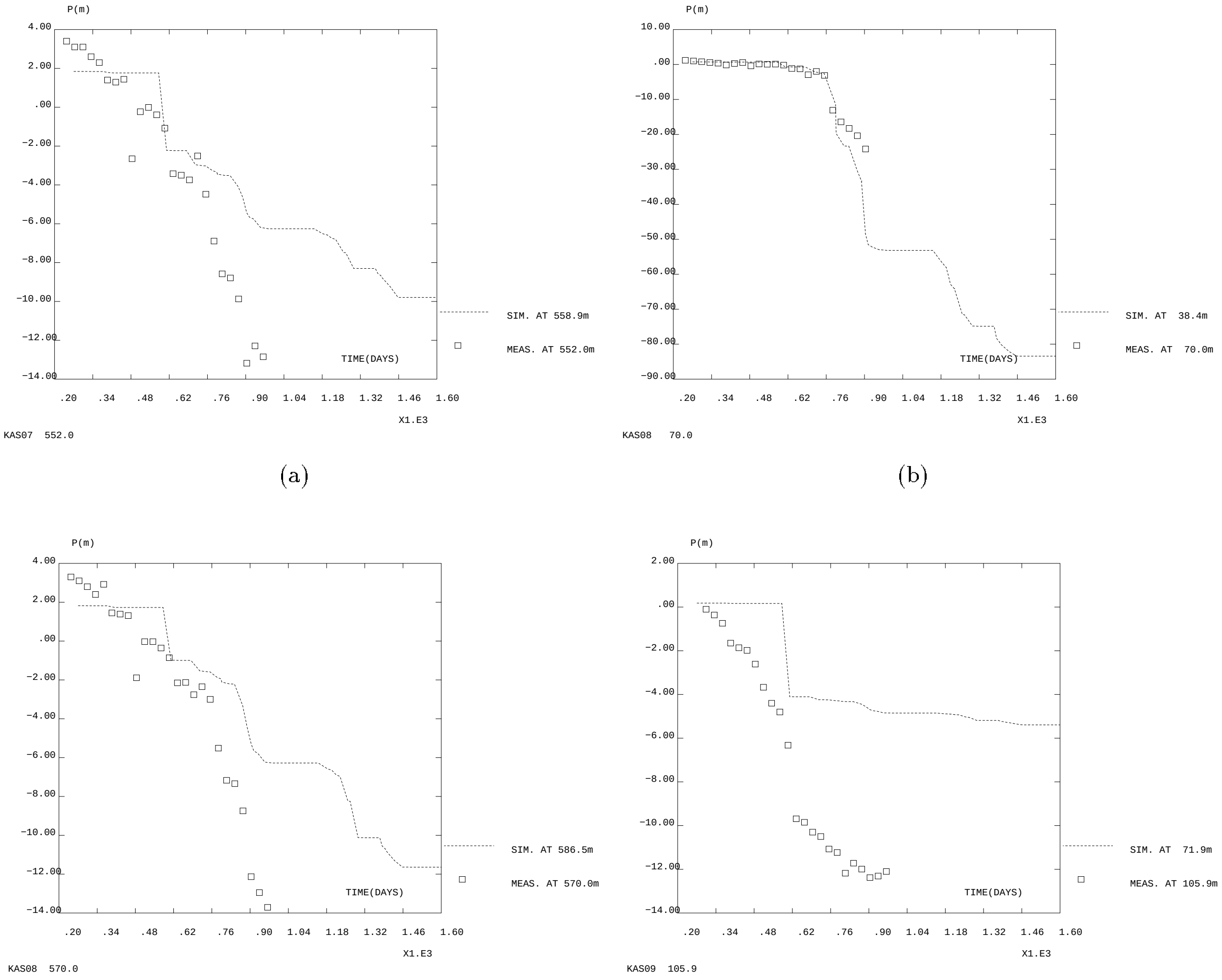
Figure 3.7: Pressures in different boreholes sections below Äspö. Measured and simulated as a function of time



(a) (b)

(c) (d)

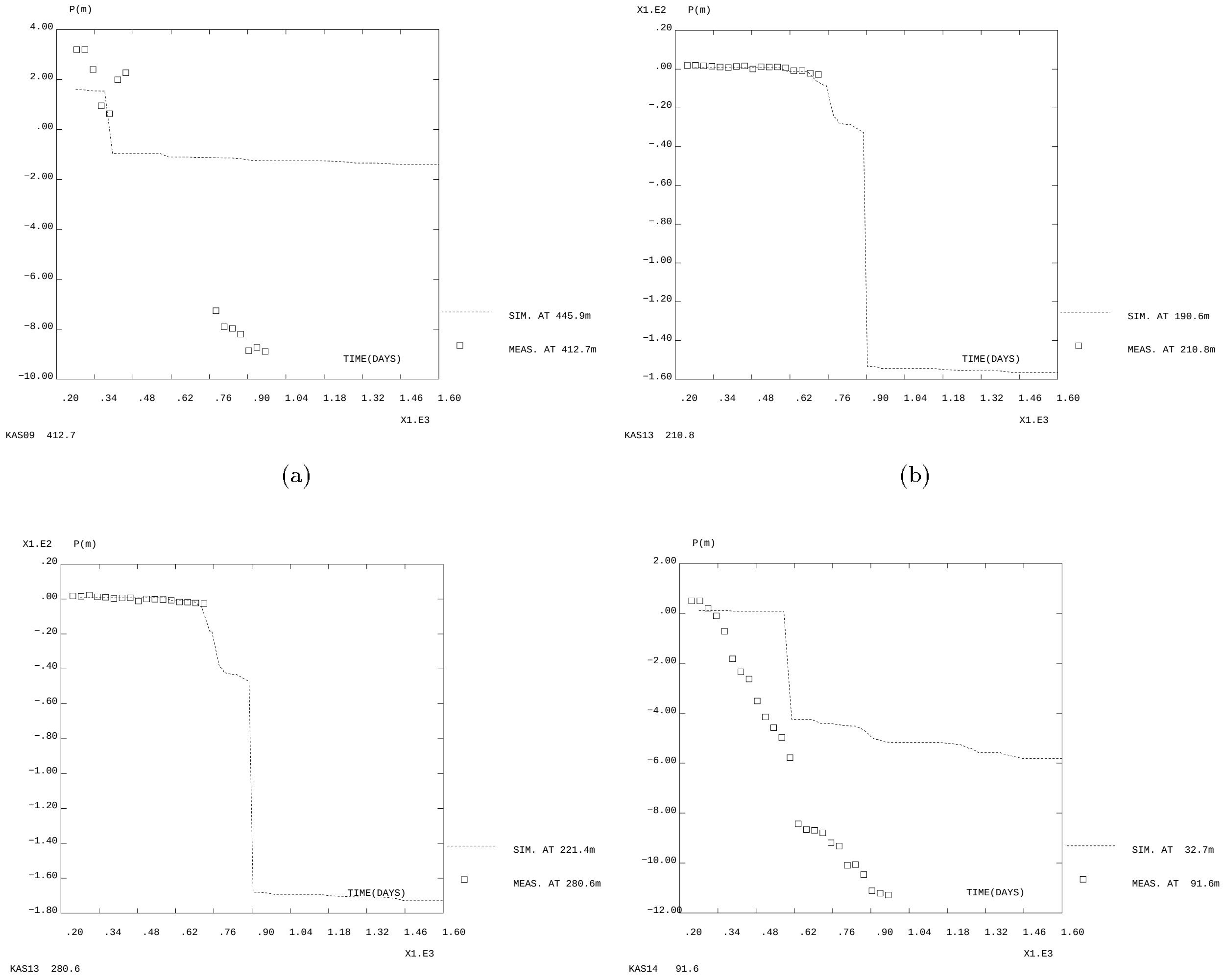
Figure 3.8: Pressures in different boreholes sections below Äspö. Measured and simulated as a function of time



(a) (b)

(c) (d)

Figure 3.9: Pressures in different boreholes sections below Äspö. Measured and simulated as a function of time



(a) (b)

(c) (d)

Figure 3.10: Pressures in different boreholes sections below Äspö. Measured and simulated as a function of time

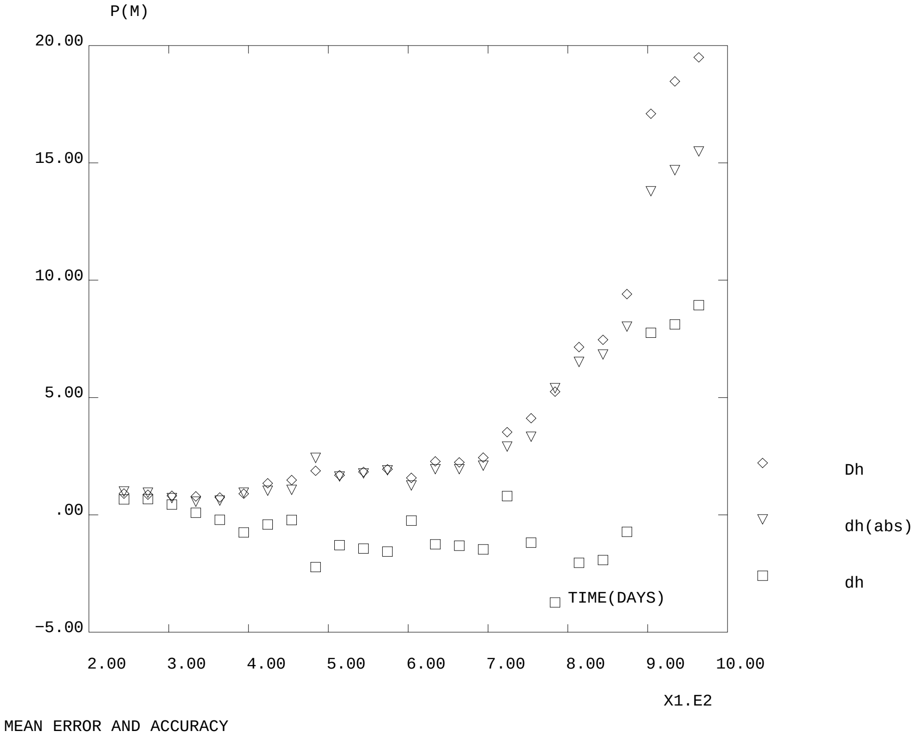
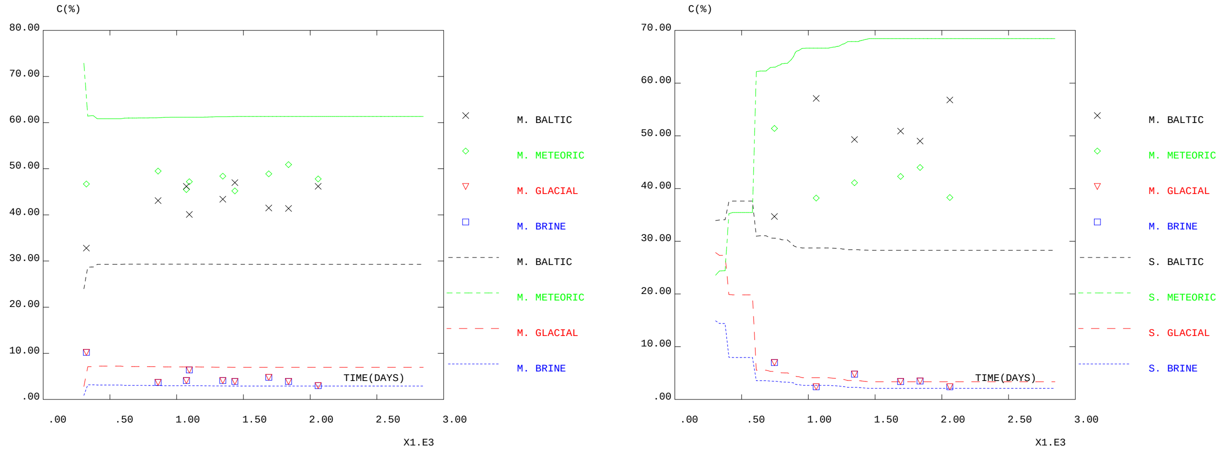


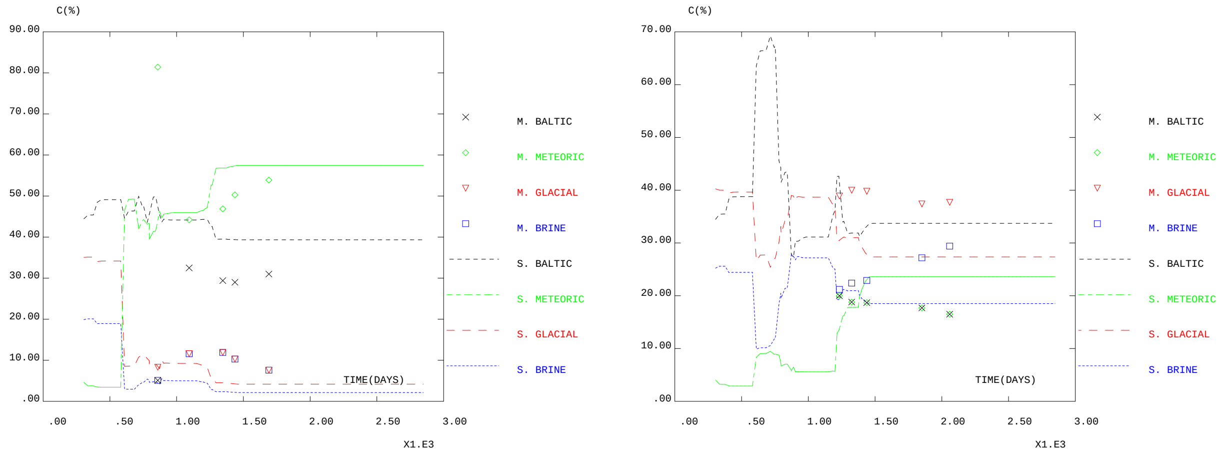
Figure 3.11: Differences between simulated and measured pressures

3.3 Mixing proportions at the control points



(a) Control point 2 (SA0813B-SA0850B)

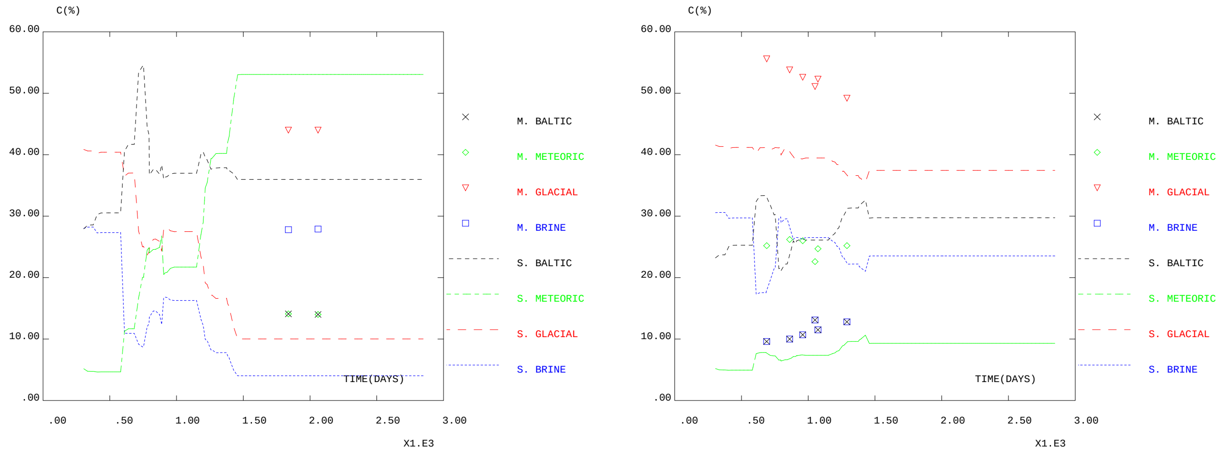
(b) Control point 3 (SA1327B-SA1229A-KA1061A)



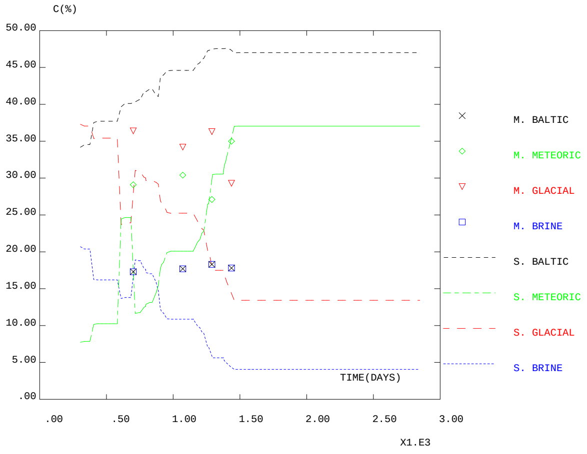
(c) Control point 4 (SA2074A)

(d) Control point 5 (SA2783A)

Figure 3.12: Mixing proportions of the four waters at control points as a function of time. Measured and simulated

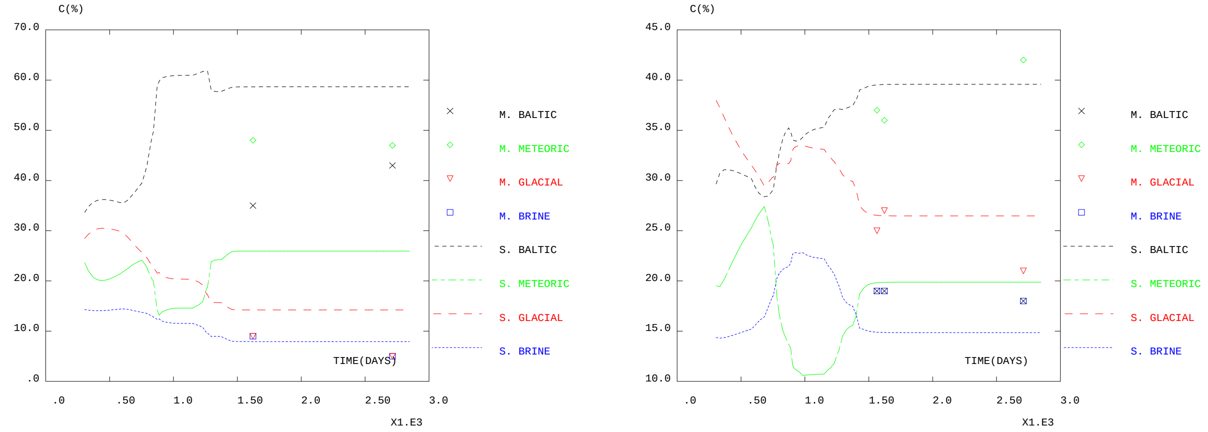


(a) Control point 6 (KA1755A) (b) Control point 10 (KAS03)



(c) Control point 11 (KAS07)

Figure 3.13: Mixing proportions of the four waters at control points as a function of time. Measured and simulated

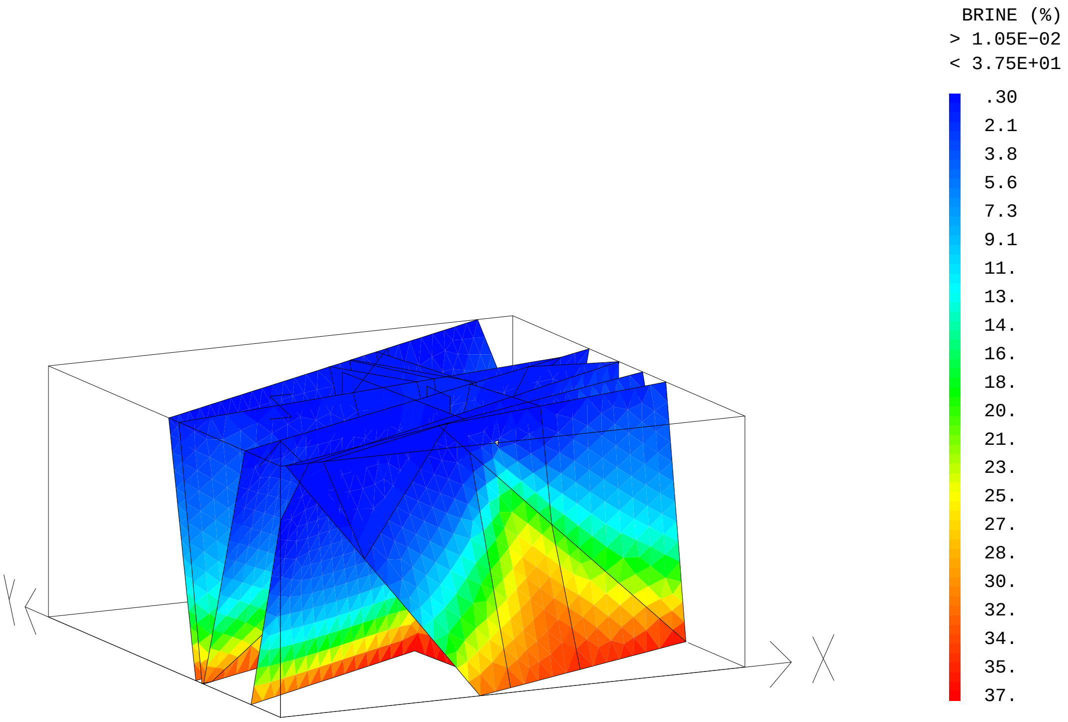


(a) Control point 8 (KA3110A) (b) Control point 9 (KA3385A)

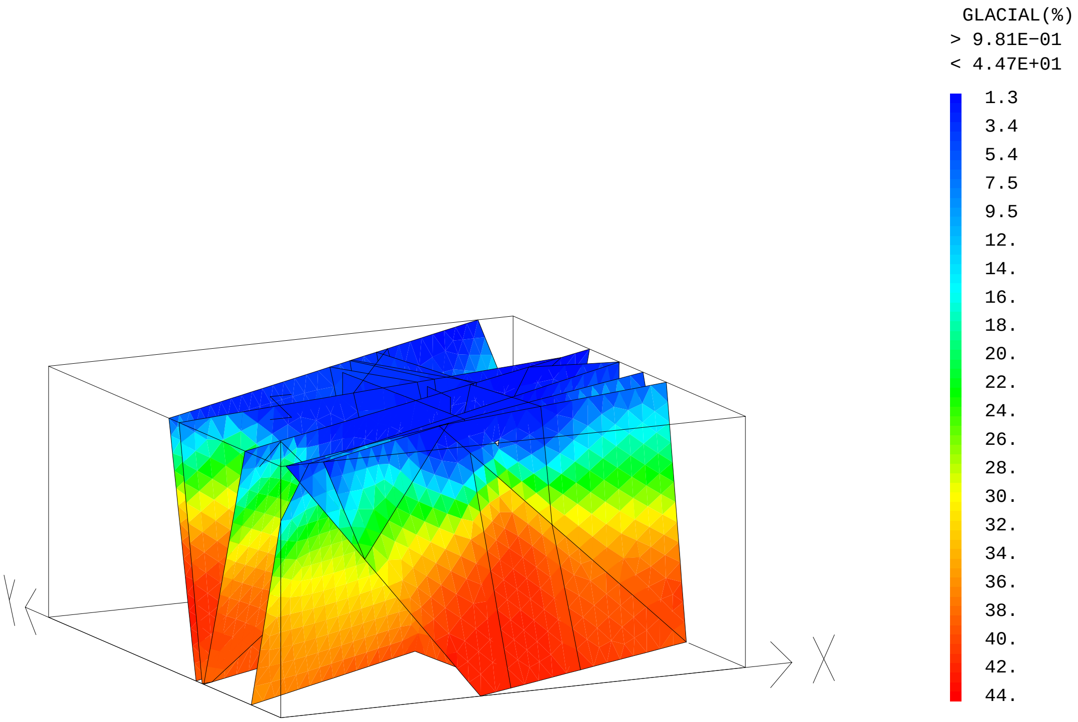
Figure 3.14: Mixing proportions of the four waters at prediction control points as a function of time. Measured and simulated

3.4 Concentration fields at different times of the excavation

The global evolution of the different waters is satisfactory : Brine and Glacial water spreading from below, Meteoric from the land and Baltic from the sea positions.

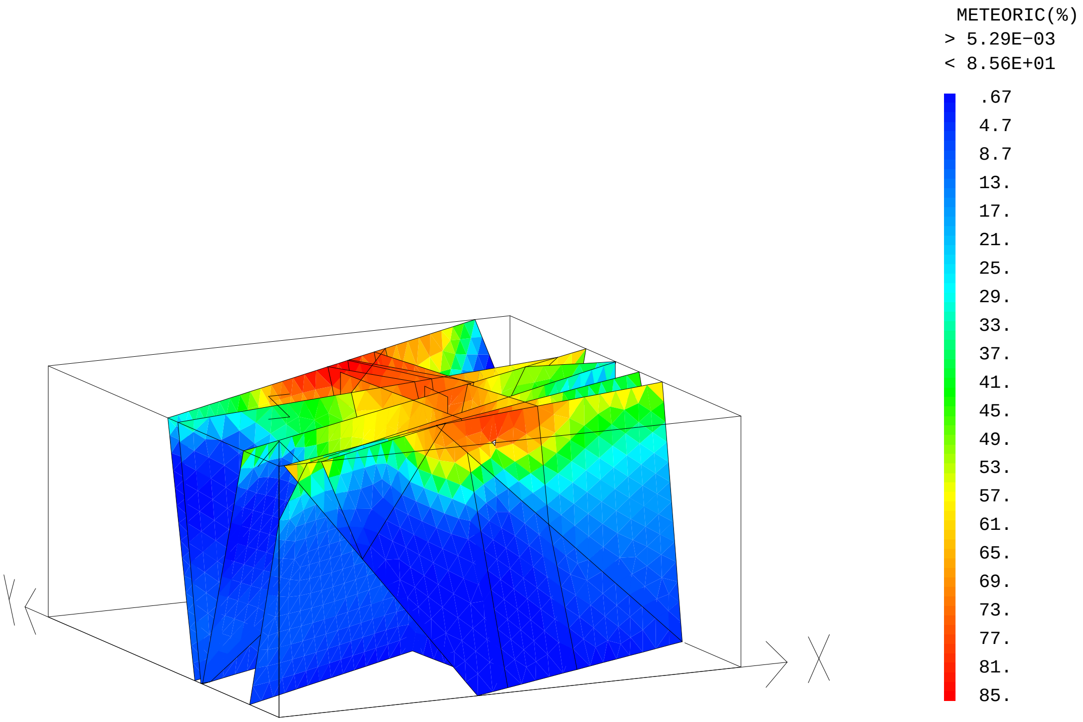


(a) Brine water proportion

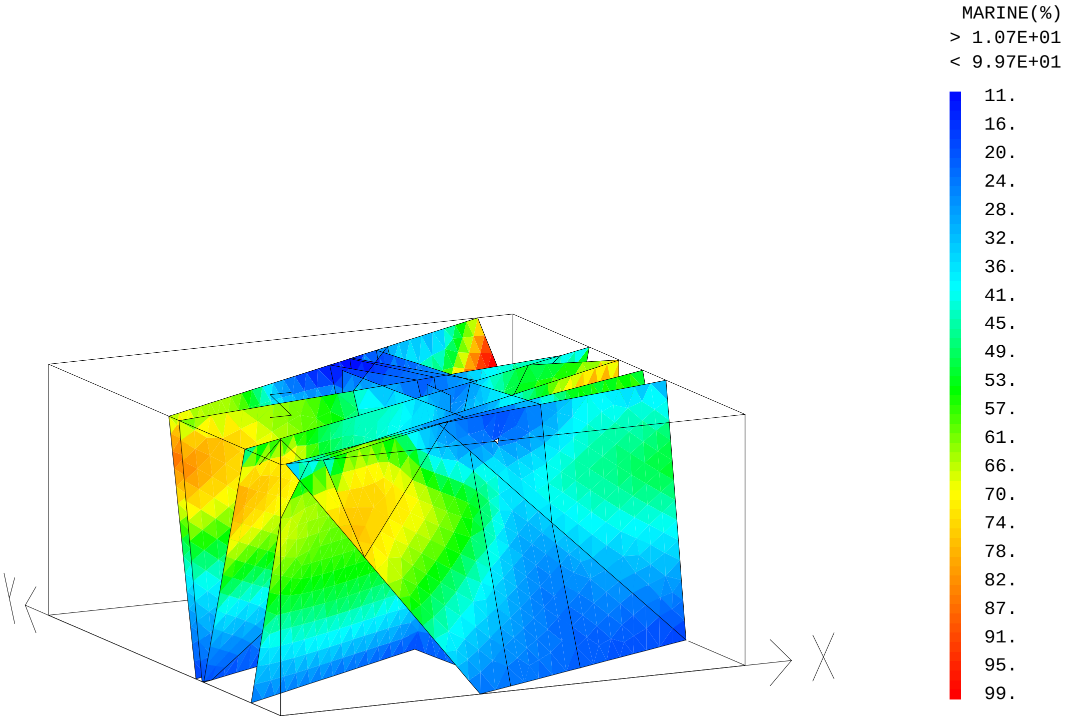


(b) Glacial water proportion

Figure 3.15: Mixing proportions of Brine and Glacial waters at time 1409 days (end of excavation)



(a) Meteoric water proportion



(b) Baltic water proportion

Figure 3.16: Mixing proportions of Meteoric and Baltic waters at time 1409 days (end of excavation)

Chapter 4

Conclusions

For the hydraulic problem, good consistency level could be achieved for the model implemented. Nevertheless, the best solution provided is not unique as shown by sensitivity analysis conducted throughout the calibration.

Incorporation of mixing proportion data into the model allows for its refinement in the sense that hydraulic calibration of the system requires improvement. Nevertheless, preliminary results based on sensitivity analysis show that further level of uncertainty are introduced taking transport data into account. These involve uncertainties in transport parameters as well as calibration data like mixing proportions obtained from M3 based on scarce measurements.

Our present level of work on the system does not allow for conclusions on global consistency of the model including hydraulic as well as transport data. Nevertheless, uncertainty concerning transport parameters as well as data are important and should be taken into account in the analysis and the calibration strategy.

From a numerical point of view, this work will leads us in the future to develop and implement in CASTEM2000 the mixed hybrid finite element formulation for flow and transport in fractured network, fractures being 2D objects. Particle tracking procedure will be adapted as well.

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[*Äspö Task Force*] : Web site under address
http://www.skb.se/omskb/forskning/aspo/tf/index.htm

Appendix A

Modeling questionnaire for TASK5

MODELLING QUESTIONNAIRE FOR TASK 5, CEA

worked October 1999

This is a Modelling Questionnaire prepared by SKB based on discussions within the Task Force group. It should be answered when reporting Task 5 in order to simplify the evaluation process of the modelling exercise. Preferably, include this response in an appendix to your forthcoming report.

1. SCOPE AND ISSUES

a) What was the purpose for your participation in Task 5? *Test our code and modelling capacities on a real test case with a good data base.*

b) What issues did you wish to address through participation in Task 5? *Flow and transport within a fractured network. Non uniqueness of the solutions for the calibration. Importance of density effects at the site. Importance of transport data with natural tracers and consistency with the different tests done.*

2. CONCEPTUAL MODEL AND DATA BASE

a) Please describe your models using the tables 1-3 in the appendix.

b) To what extent have you used the data sets delivered? Please fill in Table 4 in the appendix.

c) Specify more exactly what data in the data sets you actually used? Please fill in “Comments” in Table 4

d) What additional data did you use if any and what assumptions were made to fill in data not provided in the Data Distributions but required by your model? Please add in the last part of Table 4.

e) Which processes are the most significant for the situation at the Äspö site during the simulation period? *Hydraulic consequences of the excavation of the tunnel.*

3. MODEL GEOMETRY/STRUCTURAL MODEL

a) How did you geometrically represent the ÄSPÖ site and its features/zones? *All features are 3D, we started from 2D fractures from an automatic mesh generator (IDEAS). Finally fracture intersections are not represented but accounted for by means of continuity relations.*

b) Which features were considered the most significant for the understanding of flow and transport in the ÄSPÖ site, and why? *NE1, NE3 and NNW4 played a dominant role in the flow calibration.*

c) Motivate selected numerical discretization in relation to used values of correlation length and/or dispersion length. *Little freedom exists for the meshing, time steps had to be adjusted. In the vicinity of the tunnel and because of the importance of the velocities, precision is not optimal.*

4a. MATERIAL PROPERTIES - HYDROGEOLOGY

a) How did you represent the material properties in the hydraulic units used to represent the ÄSPÖ SITE? *Constant for each conductor domain. Grouting values affected are constant per conductor domain. Storage coefficients constant.*

b) What is the basis for your assumptions regarding material properties? *Used data provided in Rhen reports.*

c) Which assumptions were the most significant, and why?

4b. CHEMICAL REACTIONS - HYDROCHEMISTRY

a) What chemical reactions did you include? *No chemistry !*

b) What is the basis for your assumptions regarding the chosen chemical reactions?

c) Which reactions were the most significant, and why?

5a. BOUNDARY CONDITIONS FOR HYDROGEOLOGICAL MODEL

a) What boundary conditions were used in the modelling of the ÄSPÖ site tests? *The ones from Svensson regional model and were kept constant throughout the tunnel progression.*

b) What was the basis for your assumptions regarding boundary conditions? *Interpolation from a model based on a larger regional domain. The values were kept constant during the test.*

c) Which assumptions were the most significant, and why? *No sensitivity analysis was fulfilled.*

5b. BOUNDARY/INITIAL CONDITIONS FOR HYDROCHEMICAL MODEL

a) What boundary conditions were used in the modelling of the ÄSPÖ site tests? *The ones from M3 model (before and after excavation) for boundary conditions and initial conditions from M3 before excavation.*

b) What was the basis for your assumptions regarding boundary conditions? *Boundary conditions were chosen from M3 for consistency reasons since results are compared with M3 at control points. The data was interpolated from M3 grid.*

c) Which assumptions were the most significant, and why? *Behavior in the upper part of the model depends strongly on boundary conditions due to quick transfer times.*

6. MODEL CALIBRATION

a) To what extent did you calibrate your model on the provided hydraulic information? (Steady state and transient hydraulic head etc.) *First compare model with stationary results by Svensson corresponding to situation before excavation and mean transmissivities provided. Then modify transmissivity values as well as resistance values corresponding to grouting in the tunnel. Calibration was done mostly based on contributions from involved fractures to the total inflow in the different portions of the tunnel since inflows proved more sensitive than pressures in boreholes.*

b) To what extent did you calibrate your model on the provided "transport data"? (Breakthrough curves etc.) *No calibration. Only elements of sensitivity analysis.*

c) To what extent did you calibrate your model on the provided hydrochemical data? (Mixing ratios; density/salinity etc.) *Same answer.*

d) What parameters did you vary? *Elements of sensitivity to dispersivity were made and sensitivity to this parameter seems to be important. Sensitivity to boundary conditions (conditions before and after tunnel excavation).*

e) Which parameters were the most significant, and why? *Density effects proved important.*

f) Compare the calibrated model parameters with the initial data base - comments? *Calibrated and initial data base are rather consistent for the modelling work done. It seems a fair and reliable vision of the site is available.*

7. SENSITIVITY ANALYSIS

Identify the sensitivity in your model output to:

a) the discretization used : *weak for flow but stronger for transport through dispersivity values chosen.*

b) the transmissivity/hydraulic conductivity (distribution) used : *Strong for main conductors NE1 and NE3, weaker for the others.*

c) transport parameters used : *(see 6.d).*

d) chemical mixing parameters used *(not studied)*.

e) chemical reaction parameters used (not modelled).

8. LESSONS LEARNED

a) Given your experience in implementing and modelling the ÄSPÖ site, what changes do you recommend with regards to:

- Experimental site characterisation? OK
- Presentation of characterisation data? OK
- Performance measures and presentation formats? OK

b) What additional site-specific data would be required to make a more reliable prediction of the tracer experiments? *More about dispersivity and fracture variability in regional scale conducting features. Presence of non saturated flow phenomena below Äspö ?*

c) What conclusions can be made regarding your conceptual model utilised for the exercise? *It is still at a preliminary stage, and would require further calibration if time was provided. It is nevertheless sensitive to boundary and initial conditions (M3) as well as to dispersivity coefficients used.*

d) What additional generic research results are required to improve the ability to carry out predictive modelling of transport on the site scale?

9. RESOLUTION OF ISSUES AND UNCERTAINTIES

a) What inferences did you make regarding the descriptive structural-hydraulic model on the site scale for the ÄSPÖ site? *All parameters for flow and transport do not vary among the fractures which are deterministically considered and taken planar.*

b) What inference did you make regarding the active hydochemical processes, hydrochemical data provided and the hydrochemical changes calculated? *All along the line of the reports by Rhen*.

c) What issues did your model application resolve? *Importance of density effects. Fairly good consistency for the Hydraulic model.*

d) What additional issues were raised by the model application? *Improve the code in the future by including 2D features within 3D problems.*

10. INTEGRATION OF THE HYDOGEOLOGICAL AND HYDROCHEMICAL MODELLING

a) How did you integrate the hydrogeological and hydro chemical work? *Remained at a preliminary stage due to a lack of time.*

b) How can the integration of the hydrogeological and hydrochemical work be improved? *At the point where we are, mostly by moving forth and back between both models*

c) Hydrogeologist: How has the hydrochemistry contributed to your understanding of the hydrogeology around the Äspö site? *Mixing proportions provide information about the origins and travel times for the waters. These data are nevertheless uncertain.*

d) Hydrochemist: How has the hydrogeology contributed to your understanding of the hydrochemistry around the Äspö site? *We stuck to mixing proportions without chemical reactions, so that flow plays a dominant role.*

Table 1 Description of model for water flow calculations

TOPIC	Example	Our Model
Type of model	Stochastic continuum model	Deterministic
Process description	Darcy´s flow including density driven flow. (Transport equation for salinity is used for calculation of the density)	Darcy´s flow including density driven flow. (The coupling with salinity transport was made optional, calibration was done without coupling to save time). Transport of salinity fields.
Geometric framework and parameters	Model size: 1.8x1.8x1 km^3 . Deterministic features: All deterministic features provided in the data set. Rock outside the deterministic features modelled as stochastic continuum.	Model size 2x2x1km^3 Deterministic features: kept 16 : EW1S, EW3, EW7, NE1, NE2, NE3, NE4N, NE4S, NNW1, NNW2, NNW3, NNW4, NNW5, NNW6, NNW7, SFZ11. The other ones are not intersected neither by the above ones nor the tunnel and shaft. Rock outside the deterministic features is not modelled
Material properties and hydrological properties	Deterministic features: Transmissivity (T), Storativity(S) Rock outside deterministic features: Hydraulic conductivity(K), Specific storage (Ss)	Deterministic features: Transmissivity (T), Storativity(S)
Spatial assignment method	Deterministic features: Constant within each feature (T,S). No changes due to calibration. Rock outside deterministic features: (K,Ss) lognormal distribution with correlation length xx. Mean, standard deviation and correlation based on calibration of the model	Deterministic features: Constant within each feature (T,S). T values were changed during the calibration. Grouting is taken into account.
Boundary conditions	Surface: Constant flux. Sea: Constant head Vertical-North: Fixed pressure based on vertical salinity distribution. Vertical-East: Fixed pressure based on vertical salinity distribution. Vertical-South: Fixed pressure based on vertical salinity distribution. Vertical-West: Fixed pressure based on vertical salinity distribution. Bottom: No flux. Linear change by time based regional simulations for undisturbed conditions and with Äspö tunnel present.	Surface: Constant recharge on Aspo. Sea: Constant head Vertical : Head picked up from regional model by Svensson as well as salinity distributions Bottom: No flux.
Numerical tool	PHOENICS	CASTEM2000
Numerical method	Finite volume method	Mixed and Hybrid Finite Elements Method
Output parameters	Head, flow and salinity field.	Head, flow, concentration fields

Table 2 Description of model for tracer transport calculations

TOPIC	EXAMPLE	Our model
Type of model	Stochastic continuum model	Deterministic
Process description	Advection and diffusion, spreading due to spatially variable velocity and molecular diffusion.	Advection and diffusion, spreading due to spatially variable velocity and molecular diffusion.
Geometric framework and parameters	Model size: 1.8x1.8x1 km^3 . Deterministic features: All deterministic features provided in the data set. Rock outside the deterministic features modelled as stochastic continuum.	Same as for flow problem: Deterministic features: kept 16 : EW1S, EW3, EW7, NE1, NE2, NE3, NE4N, NE4S, NNW1, NNW2, NNW3, NNW4, NNW5, NNW6, NNW7, SFZ11. Rock outside the deterministic features is not modelled
Material properties	Flow porosity (ne)	Flow porosity (ne)
Spatial assignment method	ne based on hydraulic conductivity value (TR 97-06) for each cell in model, including deterministic features and rock outside these features.	ne based on hydraulic conductivity value (TR 97-06) for each cell in model
Boundary conditions	Mixing ratios for endmembers as provided as initial conditions in data sets.	Mixing ratios for endmembers as provided as initial conditions in data sets
Numerical tool	PHOENICS	CASTEM2000
Numerical method	Particle tracking method or tracking components by solving the advection/diffusion equation for each component	Transport of 4 concentration fields
Output parameters	Breakthrough curves	Concentration fields and breakthrough curves

Table 3 Description of model for chemical reactions calculations

TOPIC	EXAMPLE	Our model
Type of model	xxx	No chemical reaction was modelled
Process description	Mixing. Reactions: Xx, Yy,Zz,Dd…..	
Geometric framework and parameters	Modelling reactions within one fracture zone, NE-1.	
Reaction parameters	Xx: a=ff, b=gg,… Yy: c=. Zz: d=...	
Spatial distribution of reactions assumed	Xx: seafloor sediments Yz: Bedrock below sea, superficial Dd: Bedrock ground surface, superficial Yz: Bedrock below sea, at depth Zz: Bedrock ground surface, at depth Yy, Zz: near tunnel	
Boundary/initial conditions for the reactions	Xx: aaa… Yy: bbb…	
Numerical tool	Phreeque	
Numerical method	xx	
Output parameters	xx	

Table 4a Summary of data usage

Data del. No	Data	Importance of data (see notes)	Comment
1	Hydrochemical data 1	-	
1a	Surface bore holes- undisturbed conditions, Äspö-Laxemar	-	
1b	Surface bore holes- disturbed conditions (by tunnel excavation), Äspö	-	
1c	Surface bore holes- undisturbed conditions, Ävrö	-	
1d	Surface bore holes- sampled during drilling, Äspö	-	
1e	Data related to the Redox experiment	-	
1f	Tunnel and tunnel bore holes- disturbed conditions	-	
2	Hydogeological data 1	**P M**	
2a1	Annual mean air temperature	-	
2a2	Annual mean precipitation	p	
2a3	Annual mean evapotranspiration	p	
2b1	Tunnel front position by time	**P M**	
2b2	Shaft position by time	**P**	
2c1	Geometry of main tunnel	**P**	
2c2	Geometry of shafts	**P**	
2d	Hydrochemistry at weirs (Cloride, pH, Electrical conductivity, period: July 1993- Aug 1993)	-	
2e	Geometry of the deterministic large hydraulic features (Most of them are fracture zones)	**P**	

Table 4b Summary of data usage

Data del. No	Data	Importance of data (see notes)	Comment
3	Hydrogeological data 2		
3a	Monthly mean flow rates measured at weirs. Tunnel section 0-2900m, period May 1991 – January 1994	**P**	
3b	Piezometric levels for period June 1st 1991 – May 21st 1993. Values with 30 days interval (Task 3 data set)	**P**	
3c	Salinity levels in bore hole sections for period -Sept 1993. (Task 3 data set)	**M**	
3d	Undisturbed piezometric levels	p	
3e	Co-ordinates for bore hole sections	p	
3f	Piezometric levels for period July 1st 1990 – January 24st 1994. Daily values.	**P**p	
4	Hydochemical data 2	**PM**	
4a	Chemical components, mixing proportions and deviations for all bore hole sections used in the M3 calculations	**P**	

4b	Bore holes with time series, > 3 samples (part of 4a)	**P**	
4c	Bore holes sections interpreted to intersect deterministic large hydraulic features (Most of them are fracture zones) (part of 4a)		
4d	Chemical components, mixing proportions and deviations. Grid data based on interpolation. Undisturbed conditions	**P**	
4e	Chemical components, mixing proportions and deviations. Grid data based on interpolation. Disturbed conditions (by tunnel excavation)	**P**	
4f	Boundary and initial conditions. Chemical components, mixing proportions and deviations (1989). Grid data for vertical boundaries based on interpolation. Undisturbed conditions	**PM**	
4g	Boundary conditions after tunnel construction (1996) Chemical components, mixing proportions and deviations. Grid data for vertical boundaries based on interpolation. Disturbed conditions (by tunnel excavation)	**P**	

Table 4c Summary of data usage

Data del. No	**Data**	**Importance of data (see notes)**	**Comment**
5	Geographic data 1		
5a	Äspö coast line	-	
5b	Topography of Äspö and the nearby surroundings	-	
6	Hydro tests and tracer tests	-	
6a	Large scale interference tests (19 tests)	-	
6b	Long time pump and tracer test, LPT2	-	
7	Hydochemical data 3, update of data delivery 4 based on new endmembers. Recommended to be used instead of 4.	-	
7a	Chemical components, mixing proportions and deviations for all bore hole sections used in the M3 calculations	-	
7b	Bore holes with time series, > 3 samples (part of 7a)	-	
7c	Bore holes sections interpreted to intersect deterministic large hydraulic features (Most of them are fracture zones) (part of 7a)	-	
7d	Chemical components, mixing proportions and deviations. Grid data based on interpolation. Undisturbed	-	

	conditions		
7e	Chemical components, mixing proportions and deviations. Grid data based on interpolation. Disturbed conditions (by tunnel excavation)	-	
7f	Boundary and initial conditions. Chemical components, mixing proportions and deviations (1989). Grid data for vertical boundaries based on interpolation. Undisturbed conditions		
7g	Boundary conditions after tunnel construction (1996) Chemical components, mixing proportions and deviations. Grid data for vertical boundaries based on interpolation. Disturbed conditions (by tunnel excavation)		

Table 4d Summary of data usage

Data del. No	Data	Importance of data (see notes)	Comment
8	Performance measures and reporting 1		
8a	Performance measures		
8b	Suggested control points. 6 points in tunnel section 0-2900m and 3 point in tunnel section 2900-3600m.		
8c	Suggested flowchart for illustration of modelling		
9	Hydrogeological data 3		
9a	Monthly mean flow rates measured at weirs. Tunnel section 0-3600m, period: May 1991- Dec 1996.		
10	Geographic data 2		
10a	Topography of Äspö and the nearby surroundings (larger area than 5b)		
10b	Co-ordinates for wetlands	-	
10c	Co-ordinates for lakes	-	
10d	Co-ordinates for catchments	-	
10e	Co-ordinates for streams	-	
10f	Co-ordinate transformation Äspö system- RAK	-	
11	Boundary and initial conditions		
11a	Pressure before tunnel construction, from the regional SKB model (TR 97-09)	**M**	
11b	Salinity before tunnel construction, from the regional SKB model (TR 97-09)	**M**	
11c	Pressure after tunnel construction, from the regional SKB model (TR 97-09)	**M**	
11d	Salinity after tunnel construction, from the regional SKB model (TR 97-09)	**M**	

Table 4e Summary of data usage

Data del. No	Data	Importance of data (see notes)	Comment
12	Performance measures and reporting 2		
12a	Suggested control points. 6 points in tunnel section 0-2900m and 3 point in tunnel section 2900-3600m (same as 8b) and 2 outside the tunnel.		
13	Transport parameters compiled		
13a	LPT2 tracer tests	**P**	
13b	Tracer test during passage of fracture zone NE-1	-	
13c	Redox tracer tests	-	
13d	TRUE-1 tracer tests	-	
14	Hydrochemical data 4	-	
14a	Groundwater reactions to consider within TASK5 modelling (Description of how M3 calculates the contribution of reactions and identifying dominating reactions based on the M3 calculations.		
15	Co-ordinates for the test sections defining the control points		
16	Co-ordinates for bore holes drilled from the tunnel		

Table 4f Summary of data usage

Data del. No	Data	Importance of data (see notes)	Comment
17	Hydogeological data - prediction period		
17a	Hydrochemistry at weirs (Cloride, pH, Electrical conductivity, period: July 1993- Dec 1995)		
17b	Piezometric levels for period July 1st 1990 – Dec 1996. Daily values.		
18	Hydochemical data - prediction period.		
18a	Chemical components, mixing proportions and deviations for all bore hole sections used in the M3 calculations. Data for tunnel section 2900-3600m.		
18b	Bore holes with time series, > 3 samples (part of 18a)		
18c	Bore holes sections interpreted to intersect deterministic large hydraulic features (Most of them are fracture zones) (part of 18a)		
	Other data (part of data to Task 1, 3 and 4)		
	Fracture orientation, fracture spacing and trace length – tunnel data	**M**	
	Fracture orientation, fracture spacing– mapping of cores	**M**	
	Fracture orientation, fracture spacing and trace length – mapping of outcrops	**M**	

P = data of great importance for quantitative estimation of model parameters
p = data of less importance for quantitative estimation of model parameters
M = data of great importance used qualitatively for setting up model
m = data of less importance used qualitatively for setting up model
X = data useful as general background information
- = data not used